```
=> d his nofile

     (FILE 'HOME' ENTERED AT 15:02:27 ON 09 MAR 2007)

     FILE 'HCAPLUS' ENTERED AT 15:02:38 ON 09 MAR 2007
L1             1 SEA ABB=ON  PLU=ON  US20040175741/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 15:02:53 ON 09 MAR 2007
L2            60 SEA ABB=ON  PLU=ON  (102691-36-1/BI OR 10270-36-7/BI OR
                 103440-95-5/BI OR 140-29-4/BI OR 148582-37-0/BI OR
                 189216-59-9/BI OR 2456-81-7/BI OR 275795-11-4/BI OR
                 31680-58-7/BI OR 32316-92-0/BI OR 32909-05-0/BI OR
                 335201-49-5/BI OR 335201-53-1/BI OR 36680-46-3/BI OR
                 4546-72-9/BI OR 50-89-5/BI OR 51279-01-7/BI OR 51885-79-1/B
                 I OR 5720-07-0/BI OR 587-02-0/BI OR 612-22-6/BI OR
                 619-64-7/BI OR 702642-46-4/BI OR 702642-56-6/BI OR
                 702642-66-8/BI OR 702642-85-1/BI OR 702642-87-3/BI OR
                 702642-98-6/BI OR 702643-06-9/BI OR 702643-08-1/BI OR
                 702643-76-3/BI OR 702643-86-5/BI OR 702643-87-6/BI OR
                 702644-26-6/BI OR 748789-25-5/BI OR 748789-26-6/BI OR
                 748789-27-7/BI OR 748789-28-8/BI OR 748789-29-9/BI OR
                 748789-30-2/BI OR 748789-31-3/BI OR 748789-32-4/BI OR
                 748789-33-5/BI OR 748789-34-6/BI OR 748789-35-7/BI OR
                 748789-36-8/BI OR 748789-37-9/BI OR 748789-38-0/BI OR
                 748789-39-1/BI OR 748789-40-4/BI OR 748789-41-5/BI OR
                 748789-42-6/BI OR 748789-43-7/BI OR 748789-44-8/BI OR
                 748789-46-0/BI OR 748789-47-1/BI OR 748789-48-2/BI OR
                 951-77-9/BI OR 958-09-8/BI OR 961-07-9/BI)
L3               STR
L4               STR L3
L5             8 SEA SSS SAM L4
                 D QUE STAT
L6          1815 SEA SSS FUL L4
L7            24 SEA ABB=ON  PLU=ON  L6 AND L2
L8               STR L4
L9             0 SEA SUB=L6 SSS SAM L8
L10           36 SEA SUB=L6 SSS FUL L8
L11            9 SEA ABB=ON  PLU=ON  L10 AND L2
                 SAV L6 ISS989/A
                 SAV L10 ISS989A/A
L12            0 SEA ABB=ON  PLU=ON  L10 AND MEDLINE/LC
L13            0 SEA ABB=ON  PLU=ON  L10 AND BIOSIS/LC
L14            0 SEA ABB=ON  PLU=ON  L10 AND DRUGU/LC
L15            0 SEA ABB=ON  PLU=ON  L10 AND EMBASE/LC

     FILE 'HCAPLUS' ENTERED AT 15:25:29 ON 09 MAR 2007
L16            9 SEA ABB=ON  PLU=ON  L10

     FILE 'REGISTRY' ENTERED AT 16:05:30 ON 09 MAR 2007
L17              STR L8
L18           12 SEA SUB=L6 SSS SAM L17
L19          335 SEA SUB=L6 SSS FUL L17
L20           23 SEA ABB=ON  PLU=ON  L19 AND L2
                 SAV L19 ISS989B/A

     FILE 'HCAPLUS' ENTERED AT 16:07:04 ON 09 MAR 2007
L21          102 SEA ABB=ON  PLU=ON  L19
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L22          93 SEA ABB=ON  PLU=ON  L21 NOT L16
L23          88 SEA ABB=ON  PLU=ON  L22 AND PREP/RL
L24          81 SEA ABB=ON  PLU=ON  L23 AND (1840-2003)/PRY,AY,PY

     FILE 'REGISTRY' ENTERED AT 16:09:12 ON 09 MAR 2007
L25             STR L8
L26             STR L25
L27           2 SEA SUB=L6 SSS SAM L25
L28          84 SEA SUB=L6 SSS FUL L25
L29          18 SEA ABB=ON  PLU=ON  L28 AND L2
L30           6 SEA ABB=ON  PLU=ON  L7 NOT L29
                SAV L28 ISS989C/A

     FILE 'HCAPLUS' ENTERED AT 16:21:27 ON 09 MAR 2007
L31          28 SEA ABB=ON  PLU=ON  L28
L32          46 SEA ABB=ON  PLU=ON  BUEHLER, S?/AU
L33         406 SEA ABB=ON  PLU=ON  OTT, M?/AU
L34         934 SEA ABB=ON  PLU=ON  PFLEIDERER, W?/AU
L35           5 SEA ABB=ON  PLU=ON  (L32 OR L33 OR L34) AND (L16 OR L31)
L36           4 SEA ABB=ON  PLU=ON  L16 NOT L35
L37          19 SEA ABB=ON  PLU=ON  L31 NOT (L35 OR L36)

     FILE 'REGISTRY' ENTERED AT 16:24:38 ON 09 MAR 2007
L38           0 SEA ABB=ON  PLU=ON  L28 AND MEDLINE/LC
L39           0 SEA ABB=ON  PLU=ON  L28 AND BIOSIS/LC
L40           0 SEA ABB=ON  PLU=ON  L28 AND DRUGU/LC
L41           0 SEA ABB=ON  PLU=ON  L28 AND EMBASE/LC

     FILE 'CAOLD' ENTERED AT 16:25:17 ON 09 MAR 2007
L42           2 SEA ABB=ON  PLU=ON  L28

     FILE 'BEILSTEIN' ENTERED AT 16:25:38 ON 09 MAR 2007
L43           5 SEA ABB=ON  PLU=ON  L28


     FILE 'HCAPLUS' ENTERED AT 16:35:52 ON 09 MAR 2007
L44           3 SEA ABB=ON  PLU=ON  ("CA52:17177B"/OREF OR "CA55:5624H"/ORE
                F)
L45           2 SEA ABB=ON  PLU=ON  L44 NOT ((L35 OR L36 OR L37))

     FILE 'CAOLD' ENTERED AT 16:38:07 ON 09 MAR 2007
L46           0 SEA ABB=ON  PLU=ON  L44 NOT ((L35 OR L36 OR L37))
L47           0 SEA ABB=ON  PLU=ON  ("CA52:17177B"/OREF OR "CA55:5624H"/ORE
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     (FILE 'HOME' ENTERED AT 15:02:27 ON 09 MAR 2007)

     FILE 'HCAPLUS' ENTERED AT 15:02:38 ON 09 MAR 2007
L1             1 SEA ABB=ON  PLU=ON  US20040175741/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 15:02:53 ON 09 MAR 2007
L2            60 SEA ABB=ON  PLU=ON  (102691-36-1/BI OR 10270-36-7/BI OR
                 103440-95-5/BI OR 140-29-4/BI OR 148582-37-0/BI OR
                 189216-59-9/BI OR 2456-81-7/BI OR 275795-11-4/BI OR
                 31680-58-7/BI OR 32316-92-0/BI OR 32909-05-0/BI OR
                 335201-49-5/BI OR 335201-53-1/BI OR 36680-46-3/BI OR
                 4546-72-9/BI OR 50-89-5/BI OR 51279-01-7/BI OR 51885-79-1/B
                 I OR 5720-07-0/BI OR 587-02-0/BI OR 612-22-6/BI OR
                 619-64-7/BI OR 702642-46-4/BI OR 702642-56-6/BI OR
                 702642-66-8/BI OR 702642-85-1/BI OR 702642-87-3/BI OR
                 702642-98-6/BI OR 702643-06-9/BI OR 702643-08-1/BI OR
                 702643-76-3/BI OR 702643-86-5/BI OR 702643-87-6/BI OR
                 702644-26-6/BI OR 748789-25-5/BI OR 748789-26-6/BI OR
                 748789-27-7/BI OR 748789-28-8/BI OR 748789-29-9/BI OR
                 748789-30-2/BI OR 748789-31-3/BI OR 748789-32-4/BI OR
                 748789-33-5/BI OR 748789-34-6/BI OR 748789-35-7/BI OR
                 748789-36-8/BI OR 748789-37-9/BI OR 748789-38-0/BI OR
                 748789-39-1/BI OR 748789-40-4/BI OR 748789-41-5/BI OR
                 748789-42-6/BI OR 748789-43-7/BI OR 748789-44-8/BI OR
                 748789-46-0/BI OR 748789-47-1/BI OR 748789-48-2/BI OR
                 951-77-9/BI OR 958-09-8/BI OR 961-07-9/BI)
L3               STR
L4               STR L3
L5             8 SEA SSS SAM L4
                 D QUE STAT
L6          1815 SEA SSS FUL L4
L7            24 SEA ABB=ON  PLU=ON  L6 AND L2
L8               STR L4
L9             0 SEA SUB=L6 SSS SAM L8
L10           36 SEA SUB=L6 SSS FUL L8
L11            9 SEA ABB=ON  PLU=ON  L10 AND L2
                 SAV L6 ISS989/A
                 SAV L10 ISS989A/A
L12            0 SEA ABB=ON  PLU=ON  L10 AND MEDLINE/LC
L13            0 SEA ABB=ON  PLU=ON  L10 AND BIOSIS/LC
L14            0 SEA ABB=ON  PLU=ON  L10 AND DRUGU/LC
L15            0 SEA ABB=ON  PLU=ON  L10 AND EMBASE/LC

     FILE 'HCAPLUS' ENTERED AT 15:25:29 ON 09 MAR 2007
L16            9 SEA ABB=ON  PLU=ON  L10

     FILE 'REGISTRY' ENTERED AT 16:05:30 ON 09 MAR 2007
L17              STR L8
L18           12 SEA SUB=L6 SSS SAM L17
L19          335 SEA SUB=L6 SSS FUL L17
L20           23 SEA ABB=ON  PLU=ON  L19 AND L2
                 SAV L19 ISS989B/A

     FILE 'HCAPLUS' ENTERED AT 16:07:04 ON 09 MAR 2007
L21          102 SEA ABB=ON  PLU=ON  L19
L22           93 SEA ABB=ON  PLU=ON  L21 NOT L16
L23           88 SEA ABB=ON  PLU=ON  L22 AND PREP/RL
```

```
L24          81 SEA ABB=ON  PLU=ON  L23 AND (1840-2003)/PRY,AY,PY

     FILE 'REGISTRY' ENTERED AT 16:09:12 ON 09 MAR 2007
L25             STR L8
L26             STR L25
L27           2 SEA SUB=L6 SSS SAM L25
L28          84 SEA SUB=L6 SSS FUL L25
L29          18 SEA ABB=ON  PLU=ON  L28 AND L2
L30           6 SEA ABB=ON  PLU=ON  L7 NOT L29
                SAV L28 ISS989C/A

     FILE 'HCAPLUS' ENTERED AT 16:21:27 ON 09 MAR 2007
L31          28 SEA ABB=ON  PLU=ON  L28
L32          46 SEA ABB=ON  PLU=ON  BUEHLER, S?/AU
L33         406 SEA ABB=ON  PLU=ON  OTT, M?/AU
L34         934 SEA ABB=ON  PLU=ON  PFLEIDERER, W?/AU
L35           5 SEA ABB=ON  PLU=ON  (L32 OR L33 OR L34) AND (L16 OR L31)
L36           4 SEA ABB=ON  PLU=ON  L16 NOT L35
L37          19 SEA ABB=ON  PLU=ON  L31 NOT (L35 OR L36)

     FILE 'REGISTRY' ENTERED AT 16:24:38 ON 09 MAR 2007
L38           0 SEA ABB=ON  PLU=ON  L28 AND MEDLINE/LC
L39           0 SEA ABB=ON  PLU=ON  L28 AND BIOSIS/LC
L40           0 SEA ABB=ON  PLU=ON  L28 AND DRUGU/LC
L41           0 SEA ABB=ON  PLU=ON  L28 AND EMBASE/LC

     FILE 'CAOLD' ENTERED AT 16:25:17 ON 09 MAR 2007
L42           2 SEA ABB=ON  PLU=ON  L28

     FILE 'BEILSTEIN' ENTERED AT 16:25:38 ON 09 MAR 2007
L43           5 SEA ABB=ON  PLU=ON  L28


     FILE 'HCAPLUS' ENTERED AT 16:35:52 ON 09 MAR 2007
L44           3 SEA ABB=ON  PLU=ON  ("CA52:17177B"/OREF OR "CA55:5624H"/ORE
                F)
L45           2 SEA ABB=ON  PLU=ON  L44 NOT ((L35 OR L36 OR L37))

     FILE 'CAOLD' ENTERED AT 16:38:07 ON 09 MAR 2007
L46           0 SEA ABB=ON  PLU=ON  L44 NOT ((L35 OR L36 OR L37))
L47           0 SEA ABB=ON  PLU=ON  ("CA52:17177B"/OREF OR "CA55:5624H"/ORE
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=> d que l36
L4                STR
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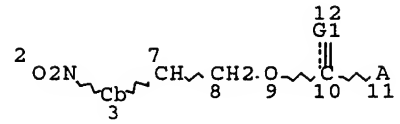


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VAR G1=O/S
NODE ATTRIBUTES:
NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L6          1815 SEA FILE=REGISTRY SSS FUL L4
L8                STR
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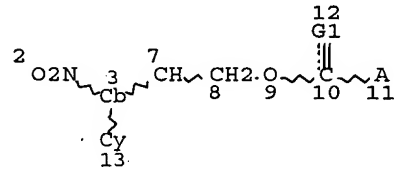


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VAR G1=O/S
NODE ATTRIBUTES:
NSPEC   IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L10           36 SEA FILE=REGISTRY SUB=L6 SSS FUL L8
L16            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10
L25               STR
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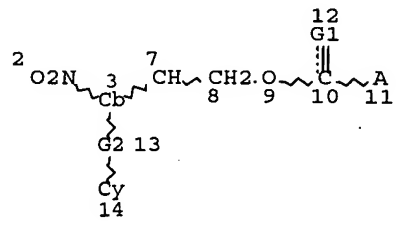
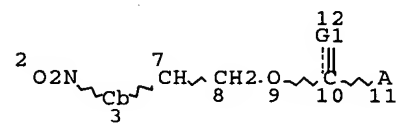


VAR G1=O/S
REP G2=(0-10) A
NODE ATTRIBUTES:
NSPEC IS RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L28 84 SEA FILE=REGISTRY SUB=L6 SSS FUL L25
L31 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L28
L32 46 SEA FILE=HCAPLUS ABB=ON PLU=ON BUEHLER, S?/AU
L33 406 SEA FILE=HCAPLUS ABB=ON PLU=ON OTT, M?/AU
L34 934 SEA FILE=HCAPLUS ABB=ON PLU=ON PFLEIDERER, W?/AU
L35 5 SEA FILE=HCAPLUS ABB=ON PLU=ON (L32 OR L33 OR L34) AND (L16 OR L31)
L36 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L35

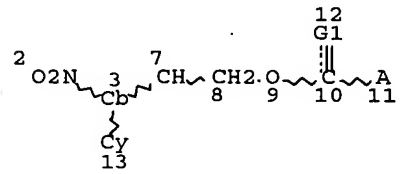
=> d que l37
L4 STR



VAR G1=O/S
NODE ATTRIBUTES:
NSPEC IS RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L6 1815 SEA FILE=REGISTRY SSS FUL L4
L8 STR

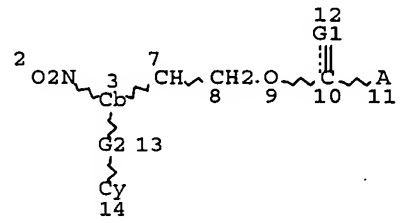


VAR G1=O/S
NODE ATTRIBUTES:
NSPEC IS RC AT 11
DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L10 36 SEA FILE=REGISTRY SUB=L6 SSS FUL L8
L16 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L10
L25 STR



VAR G1=O/S
REP G2=(0-10) A
NODE ATTRIBUTES:
NSPEC IS RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L28 84 SEA FILE=REGISTRY SUB=L6 SSS FUL L25
L31 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L28
L32 46 SEA FILE=HCAPLUS ABB=ON PLU=ON BUEHLER, S?/AU
L33 406 SEA FILE=HCAPLUS ABB=ON PLU=ON OTT, M?/AU
L34 934 SEA FILE=HCAPLUS ABB=ON PLU=ON PFLEIDERER, W?/AU
L35 5 SEA FILE=HCAPLUS ABB=ON PLU=ON (L32 OR L33 OR L34) AND (L16 OR L31)
L36 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L35
L37 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 NOT (L35 OR L36)

=> d l36 1-4 ibib ed abs hitstr hitind
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L36 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1146025 HCAPLUS Full-text
DOCUMENT NUMBER: 143:422574
TITLE: Photolabile protecting groups in synthesis of nucleosides
INVENTOR(S): Stengele, Klaus-Peter
PATENT ASSIGNEE(S): Nimblegen Systems, Inc., USA
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1589024	A1	20051026	EP 2005-8191	20050414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
DE 102004019098	A1	20051110	DE 2004-102004019098	20040420
JP 2005306873	A	20051104	JP 2005-122453	20050420
US 2005272076	A1	20051208	US 2005-109873	20050420
PRIORITY APPLN. INFO.:			DE 2004-102004019098A	20040420

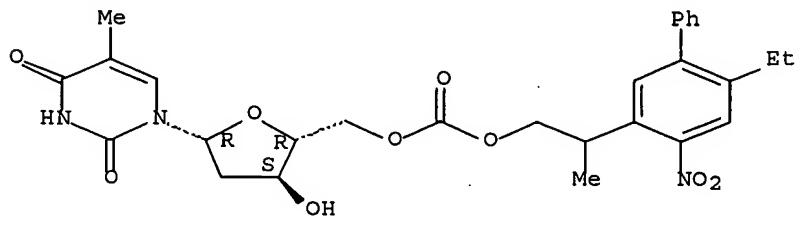
OTHER SOURCE(S): CASREACT 143:422574; MARPAT 143:422574
ED Entered STN: 27 Oct 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Nucleoside derivs. I, wherein R1 = H, halogen, NO2, CN, OCH3, alkyl, alkoxy or alkoxyalkyl residue having 1 to 4 C atoms, preferably a Me, Et, Pr or Bu residue or an optionally substituted aryl residue or aliphatic acyl residue having 2 to 5 atoms, R2 to R7 = H, NO2, CN, OCH3, a branched or unbranched alkyl, alkoxy or alkoxyalkyl residue having 1 to 5 C atoms or an optionally substituted aryl residue or an aliphatic acyl residue having 2 to 5 atoms, X is the group C = O or C = S, Y = S, O, NR', C(R')2, wherein R' is H, or a branched or unbranched alkyl residue having 1 to 5 C atoms or an optionally substituted aryl residue, Z = SO2, OCO, OCS, SCS, and Q is R or R1, B is nucleobase, R8 is H, OH, halogen, OR', SR', P = H or a protecting group common in nucleotide chemical or a common reactive group for the production of oligonucleotides, were prepared using photolabile protecting groups. Thus, nucleoside II was prepared thioxanthone as protecting group.

IT 868157-71-5
(photolabile protecting groups in synthesis of nucleosides)
RN 868157-71-5 HCAPLUS
CN Thymidine, 5'-[2-(6-ethyl-4-nitro[1,1'-biphenyl]-3-yl)propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



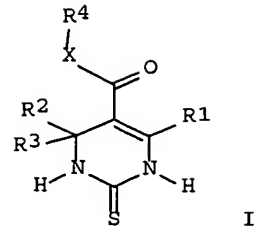
IC ICM C07H019-04
ICS C07H021-00
CC 33-9 (Carbohydrates)

IT 147-93-3 148582-37-0 189216-59-9 748789-44-8 868157-71-5
(photolabile protecting groups in synthesis of nucleosides)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1127347 HCAPLUS Full-text
DOCUMENT NUMBER: 142:74595
TITLE: Preparation of pyrimidine derivatives as hepatitis C virus inhibitors
INVENTOR(S): Lim, Jae-Hong; Yoon, Joo-Yong; Song, Jeong-Uk; Sung, Lee-Taek; Choi, Sung-Pil; Song, Ho-Young; Kim, Jong-Yup; Kim, Yong-Zu; Cho, Young-Gyu; Kim, Chang-Myung; Kim, Won-Sup; Kang, Seung-Wan; Park, Ji-Hyun
PATENT ASSIGNEE(S): LG Life Sciences Ltd., S. Korea
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004111013	A1	20041223	WO 2004-KR1370	20040609
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2004107367	A	20041220	KR 2004-40967	20040604
CA 2527851	A1	20041223	CA 2004-2527851	20040609
EP 1633725	A1	20060315	EP 2004-773898	20040609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2006527266	T	20061130	JP 2006-516915	20040609
US 2006116390	A1	20060601	US 2005-559746	20051207
PRIORITY APPLN. INFO.:			KR 2003-38246 A	20030613
			WO 2004-KR1370 W	20040609

OTHER SOURCE(S): MARPAT 142:74595
ED Entered STN: 24 Dec 2004
GI



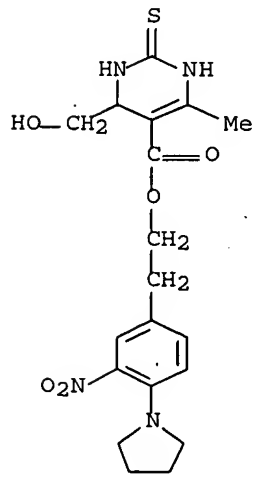
I

AB The title compds. I [X = O, S; R1 = H, (un)substituted alkyl, etc.; CR2R3 = cycloalkyl; or when one of R2 and R3 is H, the other is CH2OCOR5, etc.; R5 = (un)substituted alkyl, etc.; R4 = (un)substituted alkyl, etc.] are prepared A process for preparing I is disclosed. Thus, 6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid benzyl ester was prepared by stirring at reflux a mixture of benzyl acetoacetate, thiourea, oxazinane in acetonitrile containing trifluoroacetic acid for 6 h. Compds. of this invention showed IC50 values of 0.3 μM to > 100 μM against hepatitis C virus.

IT 813457-96-4P 813457-97-5P 813457-98-6P
(preparation of pyrimidine derivs. as hepatitis C virus inhibitors)

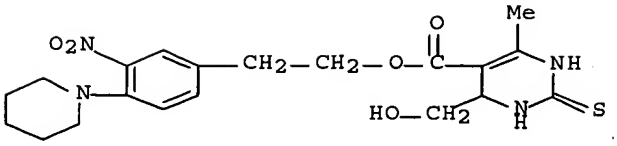
RN 813457-96-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-4-(hydroxymethyl)-6-methyl-2-thioxo-, 2-[3-nitro-4-(1-pyrrolidinyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

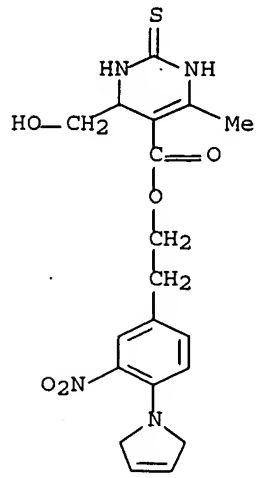


RN 813457-97-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-4-(hydroxymethyl)-6-methyl-2-thioxo-, 2-[3-nitro-4-(1-piperidinyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)



RN 813457-98-6 HCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-4-(hydroxymethyl)-6-methyl-2-thioxo-, 2-[4-(2,5-dihydro-1H-pyrrol-1-yl)-3-nitrophenyl]ethyl ester (9CI) (CA INDEX NAME)



IC ICM C07D239-10
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 10
IT 813456-07-4P 813456-08-5P 813456-09-6P 813456-10-9P
813456-11-0P 813456-12-1P 813456-13-2P 813456-14-3P
813456-15-4P 813456-16-5P 813456-17-6P 813456-18-7P
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813457-71-5P 813457-72-6P 813457-73-7P 813457-74-8P
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813457-92-0P 813457-93-1P 813457-94-2P 813457-95-3P
813457-96-4P 813457-97-5P 813457-98-6P

(preparation of pyrimidine derivs. as hepatitis C virus inhibitors)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:872740 HCAPLUS Full-text
DOCUMENT NUMBER: 141:366034
TITLE: Efficient photolithographic synthesis of DNA-chips by photosensitization
INVENTOR(S): Steiner, Ulrich; Woell, Dominik
PATENT ASSIGNEE(S): Universitaet Konstanz, Germany
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089529	A1	20041021	WO 2004-EP2361	20040308

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10315772 A1 20041104 DE 2003-10315772 20030407
PRIORITY APPLN. INFO.: DE 2003-10315772 A 20030407

OTHER SOURCE(S): MARPAT 141:366034
ED Entered STN: 21 Oct 2004

AB The present invention relates to a new chemical compound, as well as to a method of cleaving labile functional groups from mols. by electromagnetic radiation and a method of manufacturing DNA chips by spatially addressed, light controlled nucleotide synthesis on solid substrates. This invention provides a chemical compound which comprises the structural motif S-(LI)a-P-(L2)b-R, wherein S represents a sensitizer synthon, which first excited electronic state is energetically higher than the first excited electronic state of the labile functional group P (also termed as "protecting group synthon"). The presence of conjugated 7r-systems or conjugated double bonds is especially preferred. It is important, that the sensitizer synthon comprises at least three conjugated double bonds. After excitation of the sensitizer synthon by irradiation of suitable wavelength, the sensitizer synthon changes via intersystem crossing (ISC) from an excited singlet state in the triplet system and relaxes in the lowest excited triplet state. It is understood, that the same applies for every other protecting group synthon, like benzophenone or thioxanthone derivs. The energy of the triplet state is transferred via triplet triplet energy transfer to the protecting group synthon, where by the sensitizer synthon and the protecting group synthon are linked by a bridge. After transfer of the energy to the protecting group synthon, the cleavage of the bond between the substrate and the photolabile protecting group (location C) occurs, so that the substrate can be used selectively for further reactions. Conditions and kinetics of triplet sensitization as a method for increasing the light sensitivity of photolabile protecting groups used for the photolithog. synthesis of oligonucleotide microarrays were quant. studied with the photolabile 2-(2-nitrophenyl)propyl protecting group in homogeneous solns. and on glass substrates by using laser flash photolysis, continuous illumination with HPLC anal., fluorescence dye labeling, and hybridization. It was further demonstrated that, with 9H-thioxanthen-9-one as a sensitizer, high-d. oligonucleotide microarrays of high quality can be produced with one-third of the normal exposure time.

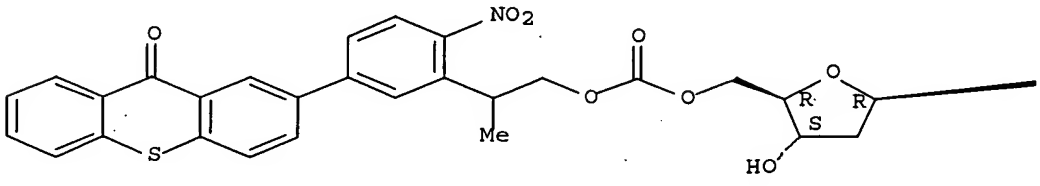
IT **777864-78-5P**, 5-O'-[2-[5-(9-Oxo-9H-thioxanthen-2-yl)-2-nitrophenyl]propoxycarbonyl]thymidine
(photolithog. synthesis of DNA-chips by photosensitization)

RN 777864-78-5 HCAPLUS

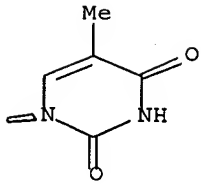
CN Thymidine, 5'-[2-[2-nitro-5-(9-oxo-9H-thioxanthen-2-yl)phenyl]propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



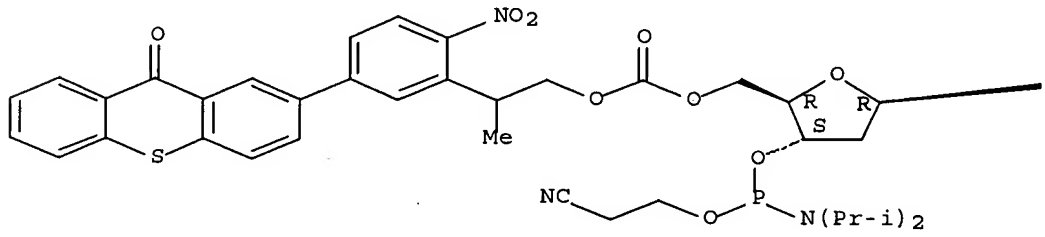
PAGE 1-B



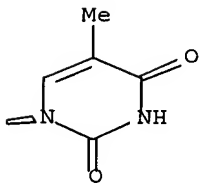
IT 777864-79-6P
(photolithog. synthesis of DNA-chips by photosensitization)
RN 777864-79-6 HCAPLUS
CN Thymidine, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] 5'-[2-[2-nitro-5-(9-oxo-9H-thioxanthen-2-yl)phenyl]propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



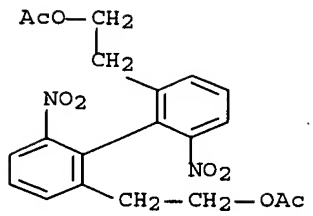
IC ICM B01J019-00
ICS C07H019-00; C07H021-00
CC 25-22 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 3, 74
IT 31696-67-0P, 2-Hydroxy-9H-thioxanthen-9-one 103440-95-5P, 4-Ethyl-3-nitrobenzoic acid 193087-05-7P, 2-Iodo-9H-thioxanthen-9-one 274676-13-0P 702642-66-8P, 4-Ethyl-3-nitrobenzoic acid tert-butyl ester 702643-08-1P, 2-(4-tert-Butoxycarbonyl-2-nitrophenyl)propanol 777864-66-1P, 2-(2-Nitrophenyl)pent-4-ynoic acid methyl ester 777864-67-2P, 2-(2-Nitrophenyl)-4-pentyn-1-ol 777864-68-3P, 2-(2-Nitrophenyl)-5-(9-oxothioxanthen-2-yl)-4-pentyn-1-ol 777864-69-4P, 5'-O-[2-(Nitrophenyl)-5-(9-oxothioxanthen-2-yl)pent-

4-ynyloxycarbonyl]thymidine 777864-70-7P, 4-[2-(2-Methoxyethoxymethoxy)-1-methylethyl]-3-nitrobenzoic alcohol acid tert-butyl ester 777864-71-8P, 4-[2-(2-Methoxyethoxymethoxy)-1-methylethyl]-3-nitrobenzoic acid 777864-73-0P, 4-[2-(2-Methomyethoxymetholoy)-1-methylethyl]-3-nitrobenzoic acid 9-oxo-9H-thioamnthen-2-yl ester 777864-74-1P, 4-(2-Hydroxy-1-methylethyl)-3-nitrobenzoic acid 9-oxo-9H-thioxanthen-2-yl ester 777864-76-3P, 2-(5,5-Dimethyl-1,3,2-dioxaborinan-2-yl)-9H-thioxanthen-9-one 777864-77-4P, 2-[3-(1-Hydroxyprop-2-yl)-4-nitrophenyl]-9H-thioxanthen-9-one **777864-78-5P**, 5-O'-[2-[5-(9-Oxo-9H-thioxanthen-2-yl)-2-nitrophenyl]propoxycarbonyl]thymidine 777864-80-9P, 2-(2-Nitrophenyl)pent-4-en-1-ol 777864-83-2P, 2-[5-(tert-Butyldimethylsilyl)oxy-4-(2-nitrophenyl)pentyl]-9H-thioxanthen-9-one 777864-84-3P, 2-[5-Hydroxy-4-(2-nitrophenyl)pentyl]-9H-thioxanthen-9-one 777864-86-5P
(photolithog. synthesis of DNA-chips by photosensitization)

IT 777864-75-2P, 5-O'-[2-[4-(9-Oxo-9H-thioxanthen-2-yl)carbonyl-2-nitrophenyl]propoxycarbonyl]thymidine **777864-79-6P**
777864-81-0P, 1-[(tert-Butyldimethylsilyl)oxy]-2-(2-nitrophenyl)pent-4-ene 855743-26-9P, 5'-O-[(2-Nitrophenyl)-5-(9-oxo-9H-thioxanthen-2-yl)pentyloxyearbonyl]thymidine
(photolithog. synthesis of DNA-chips by photosensitization)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

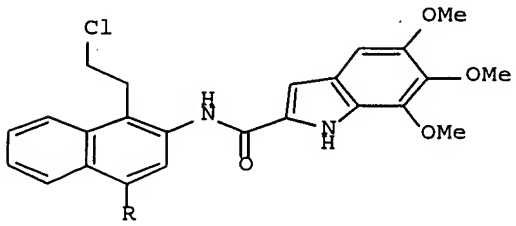
L36 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:112771 HCAPLUS Full-text
DOCUMENT NUMBER: 102:112771
TITLE: Synthesis and chiroptical properties of bridged 2,2'-diaminobiphenyl derivatives
AUTHOR(S): Seno, Kaoru; Hagishita, Sanji; Sato, Tomohiro; Kuriyama, Kaoru
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi Co., Osaka, 553, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (9), 2013-22
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:112771
ED Entered STN: 06 Apr 1985
GI For diagram(s), see printed CA Issue.
AB The relationship between CD spectra and conformation of chiral 2,2'-diaminobiphenyls was studied as a function of the torsion angle between the ring planes. The structures of benzazocinobenzazocine [(S)-(+)-I], (S)-(-)-2,6-Me(H2N)C6H3C6H3(NH2)Me-2,6 (II) and dibenzodiazocine III were determined by x-ray crystallog. The shape of the CD spectrum of I is similar to those of II and III. The exptl. results and theor. consideration by the exciton and π-SCF MO approxns. showed that the shape of the CD spectrum is the same at least for torsion angles of 0-120°. The shape of the CD spectrum of the protonated species was inverted, with a critical torsion angle of .apprx.90°.
IT **95067-37-1P**
(preparation and hydrolysis of)
RN 95067-37-1 HCAPLUS
CN [1,1'-Biphenyl]-2,2'-diethanol, 6,6'-dinitro-, diacetate (ester) (9CI) (CA INDEX NAME)



CC 22-11 (Physical Organic Chemistry)
Section cross-reference(s): 25, 28, 75
IT 67992-16-9P 95067-29-1P 95067-34-8P 95067-37-1P
95067-40-6P 95067-42-8P
(preparation and hydrolysis of)

=> d l37 1-19 ibib ed abs hitstr hitind
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L37 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:456759 HCAPLUS Full-text
DOCUMENT NUMBER: 145:124404
TITLE: Efficient Synthesis of Achiral seco-Cyclopropylbenz[2,3-e]indoline Analogues: [4-Amino-2-(5,6,7-trimethoxyindole-2-carboxamido)naphthalen-1-yl]ethyl Chloride and [4-Hydroxy-2-(5,6,7-trimethoxyindole-2-carboxamido)naphthalen-1-yl]ethyl Chloride
AUTHOR(S): Sato, Atsushi; Scott, Adrienne; Asao, Tetsuji; Lee, Moses
CORPORATE SOURCE: Department of Chemistry, Furman University, Greenville, SC, 29613, USA
SOURCE: Journal of Organic Chemistry (2006), 71(12), 4692-4695
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124404
ED Entered STN: 17 May 2006
GI



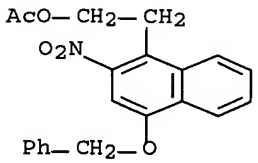
I

AB The significantly improved synthetic strategies for preparation of indolecarboxamides I (R = H2N, HO) as achiral seco- aminocyclopropylbenz[2,3-e]indoline and seco- hydroxycyclopropylbenz[2,3-e]indoline (seco-CBI) analogs of the duocarmycins and CC-1065 useful as anticancer agents are reported. Starting from 2,4-dinitro-1-naphthol (Martius acid), the new strategy gave a 13-fold increase in the overall yield of I (R = H2N), and the use of di-tert-Bu malonate was economically beneficial. For I (R = HO), the strategy employed an Emmons-Horner reaction followed by Stobbe condensation, and the overall yield was improved 15-fold.

IT **413578-23-1P 897918-34-2P**
(efficient synthesis of N-naphthyl (trimethoxy)indolecarboxamides as achiral seco-cyclopropylbenz[2,3-e]indoline analogs)

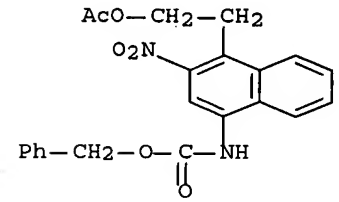
RN 413578-23-1 HCAPLUS

CN 1-Naphthaleneethanol, 2-nitro-4-(phenylmethoxy)-, acetate (ester) (9CI) (CA INDEX NAME)



RN 897918-34-2 HCAPLUS

CN Carbamic acid, [4-[2-(acetyloxy)ethyl]-3-nitro-1-naphthalenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

IT 2401-85-6P, 1-Chloro-2,4-dinitronaphthalene 261957-14-6P
413577-65-8P 413577-67-0P 413577-69-2P 413577-71-6P
413577-73-8P 413577-75-0P 413577-79-4P 413577-81-8P
413577-85-2P 413577-89-6P 413578-20-8P 413578-21-9P
413578-22-0P **413578-23-1P** 413578-25-3P 413578-26-4P
413578-27-5P 413578-28-6P **897918-34-2P** 897918-35-3P
897918-36-4P 897918-37-5P 897918-38-6P 897918-39-7P
897918-40-0P 897918-41-1P 897918-42-2P 897918-43-3P
897918-44-4P 897918-45-5P 897918-46-6P 897918-47-7P
(efficient synthesis of N-naphthyl (trimethoxy)indolecarboxamides as achiral seco-cyclopropylbenz[2,3-e]indoline analogs)

REData is temporarily unavailable.

L37 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

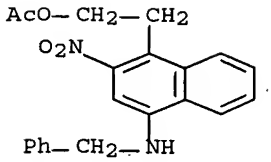
ACCESSION NUMBER: 2005:383225 HCAPLUS Full-text
DOCUMENT NUMBER: 143:70994
TITLE: A Novel Class of in Vivo Active Anticancer Agents: Achiral seco-Amino- and seco-Hydroxycyclopropylbenz[e]indolone (seco-CBI) Analogues of the Duocarmycins and CC-1065
AUTHOR(S): Sato, Atsushi; McNulty, LuAnne; Cox, Kari; Kim, Susan; Scott, Adrienne; Daniell, Kristen; Summerville, Kaitlin; Price, Carly; Hudson, Stephen; Kiakos, Konstantinos; Hartley, John A.; Asao, Tetsuji; Lee, Moses
CORPORATE SOURCE: Department of Chemistry, Furman University, Greenville, SC, 29613, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(11), 3903-3918
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:70994
ED Entered STN: 05 May 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

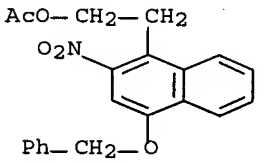
AB One achiral seco-hydroxycyclopropylbenz[e]indolone (seco-CBI) (I) and seven achiral seco-amino-CBI analogs of CC-1065 and the duocarmycins (e.g. II) were designed, synthesized and evaluated for their DNA-binding and anticancer properties. These compds. contain a core 2-chloroethylnaphthalene structure and they do not have a stereo-center. From thermal cleavage gel analyses, the seven achiral compds. and I demonstrated similar covalent sequence specificity to adozelesin and the racemic seco-CBI-TMI (III) for binding to the 5'-AAAAA(865)-3' site. Continuous exposure of human (K562) and murine (B16, L1210 and P815) cancer cell lines to the compds. demonstrated their significant cytotoxicity, with IC50 values in the sub-micromolar range. Generally, a good leaving group on the Et moiety and a free amino or hydroxyl group on the naphthyl moiety are essential for activity. According to NCI's cytotoxicity screen, compds. II and I were active against human cancer cell lines derived from lung, colon, melanoma, renal system, and breast. At the resp. doses of 15 and 20 mg/kg (administered via an i.p. route), compds. II and I inhibited the growth of murine B16-F0 melanoma in C57BL/6 mice, with minimal toxicity, and II gave a significant anticancer effect. The in vivo anticancer activity of compound II was confirmed in a human tumor xenograft study (advanced stage SC-OVCAR-3 ovarian cancer growing in scid mice). Finally, compound II was not toxic to murine bone marrow cell growth in culture at a dose that was toxic for the previously reported compound III.

IT **855299-63-7**
(novel class of in vivo active anticancer agents and achiral seco-amino- and seco-hydroxycyclopropylbenz[e]indolone (seco-CBI) analogs of duocarmycins and CC-1065)

RN 855299-63-7 HCAPLUS
CN 1-Naphthaleneethanol, 2-nitro-4-[(phenylmethyl)amino]-, acetate (ester) (9CI) (CA INDEX NAME)



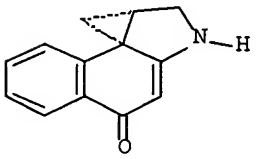
IT 413578-23-1P
(novel class of in vivo active anticancer agents and achiral seco-amino- and seco-hydroxycyclopropylbenz[e]indolone (seco-CBI) analogs of duocarmycins and CC-1065)
RN 413578-23-1 HCAPLUS
CN 1-Naphthaleneethanol, 2-nitro-4-(phenylmethoxy)-, acetate (ester) (9CI) (CA INDEX NAME)



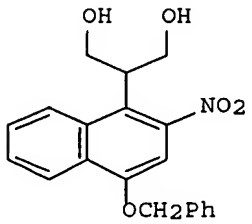
CC 1-3 (Pharmacology)
Section cross-reference(s): 27
IT 2401-85-6 4382-54-1 32864-38-3 110314-42-6 128781-07-7
173088-63-6 413578-00-4 855299-63-7
(novel class of in vivo active anticancer agents and achiral seco-amino- and seco-hydroxycyclopropylbenz[e]indolone (seco-CBI) analogs of duocarmycins and CC-1065)
IT 413577-65-8P 413577-67-0P 413577-69-2P 413577-96-5P
413577-97-6P 413577-98-7P 413578-01-5P 413578-03-7P
413578-05-9P 413578-07-1P 413578-20-8P 413578-21-9P
413578-22-0P 413578-23-1P 413578-24-2P 413578-25-3P
413578-26-4P 413578-27-5P 855299-60-4P 855299-61-5P
855299-62-6P 855299-65-9P 855299-66-0P 855299-67-1P
855299-68-2P 855299-69-3P 855299-70-6P 855299-71-7P
855299-72-8P 855299-73-9P 855299-74-0P 855299-75-1P
855299-76-2P 855299-77-3P 855299-78-4P 855299-79-5P
855299-80-8P 855299-81-9P 904664-11-5P
(novel class of in vivo active anticancer agents and achiral seco-amino- and seco-hydroxycyclopropylbenz[e]indolone (seco-CBI) analogs of duocarmycins and CC-1065)
REData is temporarily unavailable.

L37 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:183403 HCAPLUS Full-text
DOCUMENT NUMBER: 140:375040
TITLE: Effective Asymmetric Synthesis of 1,2,9,9a-Tetrahydrocyclopropa[c]benzo[e]indol-4-one (CBI)
AUTHOR(S): Kastrinsky, David B.; Boger, Dale L.
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute

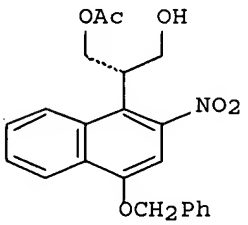
for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Organic Chemistry (2004), 69(7), 2284-2289
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:375040
ED Entered STN: 08 Mar 2004
GI



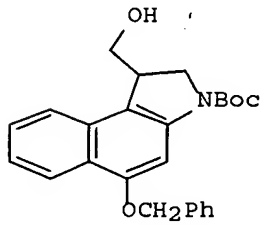
I



II



III



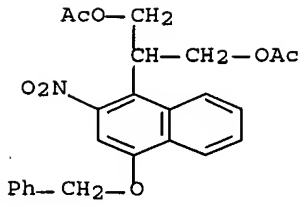
IV

AB A short, asym. synthesis of the 1,2,9,9a-tetrahydrocyclopropa[c]benzo[e]indol-4-one (CBI; I) analog of the CC-1065 and duocarmycin alkylation subunits is detailed that employs an effective enzymic desymmetrization reaction of prochiral diol II using a com. available Pseudomonas sp. lipase. The optically active monoacetate (S)-III is furnished in exceptional conversions (88%) and optical purity (99% ee) and serves as an intermediate for the preparation of either enantiomer of CBI. Similarly, the Pseudomonas sp. lipase resolved the racemic intermediate IV, affording advanced intermediates of CBI in good conversions and optical purity (99% ee), and provided an alternative approach to the preparation of optically active CBI derivs.

IT **685142-91-0P**
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)

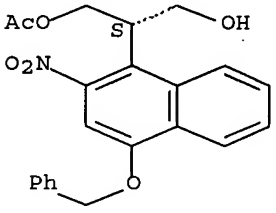
RN 685142-91-0 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)-1-naphthalenyl]-, diacetate (ester) (9CI) (CA INDEX NAME)



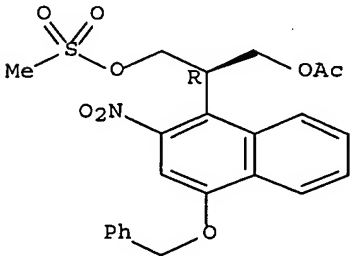
IT 685142-90-9P
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)
RN 685142-90-9 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)-1-naphthalenyl]-, monoacetate (ester), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 685142-92-1P
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)
RN 685142-92-1 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)-1-naphthalenyl]-, acetate (ester) methanesulfonate (ester), (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



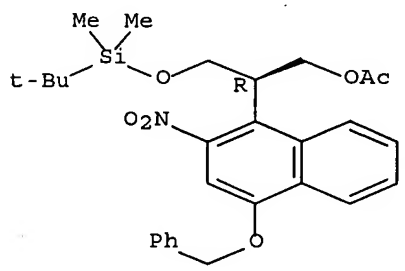
IT 685142-96-5P

(enantioselective preparation of dihydrobenzoindoles as advanced intermediates for unnatural enantiomer of CBI via orthogonal protection of enantiopure naphthalenylpropanol followed by acetate hydrolysis, mesylation and cyclization)

RN 685142-96-5 HCAPLUS

CN 1-Naphthaleneethanol, β-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-nitro-4-(phenylmethoxy)-, acetate (ester), (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



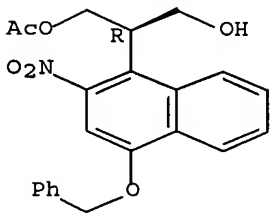
IT 685143-10-6P

(enantioselective preparation of monoacetate of naphthalenylpropanediol as chiral precursor for CBI via Pseudomonas sp. lipase catalyzed deacylation resolution of the corresponding diacetate)

RN 685143-10-6 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)-1-naphthalenyl]-, monoacetate (ester), (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

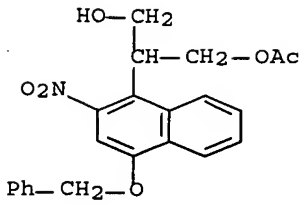


IT 685142-89-6P

(preparation of racemic monoacetate of benzyloxynitronaphthalenylpropanediol as reference sample via acetylation of the diol with acetic anhydride)

RN 685142-89-6 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)-1-naphthalenyl]-, monoacetate (ester) (9CI) (CA INDEX NAME)



CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
IT **685142-91-0P**
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)
IT **685142-90-9P** 685143-05-9P
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)
IT **685142-92-1P** 685142-93-2P 685142-94-3P 685143-04-8P
(enantioselective preparation of butyloxycarbonyldihydrobenzoindoles as precursor for enantiomeric CBI via Pseudomonas sp. lipase catalyzed enzymic acetylation of naphthalenylpropanediol with vinyl acetate as a key step)
IT 128300-12-9P **685142-96-5P** 685142-97-6P 685142-98-7P
685142-99-8P 685143-00-4P 685143-06-0P 685143-07-1P
685143-08-2P
(enantioselective preparation of dihydrobenzoindoles as advanced intermediates for unnatural enantiomer of CBI via orthogonal protection of enantiopure naphthalenylpropanol followed by acetate hydrolysis, mesylation and cyclization)
IT **685143-10-6P**
(enantioselective preparation of monoacetate of naphthalenylpropanediol as chiral precursor for CBI via Pseudomonas sp. lipase catalyzed deacylation resolution of the corresponding diacetate)
IT **685142-89-6P**
(preparation of racemic monoacetate of benzyloxynitronaphthalenylpropane diol as reference sample via acetylation of the diol with acetic anhydride)
REData is temporarily unavailable.

L37 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:300621 HCAPLUS Full-text
DOCUMENT NUMBER: 138:321053
TITLE: Methods of preparation of achiral analogs of CC-1065 and the duocarmycins and compositions thereof for use in cancer therapy
INVENTOR(S): Lee, Moses
PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 65 pp., Cont.-in-part of U.S. Ser. No. 666,160.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073731	A1	20030417	US 2001-955062	20010919
US 6660742	B2	20031209		
ES 2254492	T3	20060616	ES 2001-1973146	20010919
PRIORITY APPLN. INFO.:			US 2000-666160 A2	20000919

OTHER SOURCE(S): MARPAT 138:321053
ED Entered STN: 18 Apr 2003
GI

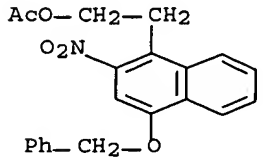
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to novel achiral seco-analogs of the DNA minor groove and sequence-selective alkylating agents (+)-CC1065 and the duocarmycins, depicted as general class I [R = CH2Ph, CO2CH2Ph, H, CO2CH2C6H4NO2-4, (4-methylpiperazin-1-yl)carbonyl; R1 = suitable minor groove binding agent, OCMe3, OCH2Ph, 9-fluorenylmethoxy, N-protecting group; R2, R3 = H, (un)branched C1-5-alkyl (e.g., Et, CH2Et, Bu, pentyl, hexyl), preferably R2 = R3 =H; R4, R5 = H, short chain alkyl, alkoxycarbonyl, preferably CO2Me, CF3; X = leaving group (Cl, Br, I, OSO2Me, OSO2C6H4Me-4, OAc, quaternary ammonium moiety, SH, C1-6-alkylsulfoxyl, C1-6-alkylsulfonyl, preferably Cl, Br, I)], II, III, IV and V. Thus, seco-analog VI was prepared from N-methyl-4-(N-methyl-4-nitropyrrole-2-carboxamido)pyrrole-2- carboxylate via hydrogenation, acylation with butyryl chloride, saponification and alkylation with 2-(2-amino-4-hydroxyphenyl)ethyl chloride. The present invention is further directed to pharmaceutical compns. thereof, and as a method for treatment of cancer using the subject compds. The cytotoxicity of VI was determined [IC50 = 12.1 μM vs. K562 leukemia cells after 1 h; IC50 = 18.0 μM vs. human colon LS174T cells after 1 h; IC50 = 82.4 μM vs. human prostate PC3 cells after 1 h; IC50 = >50.0 μM vs. human breast MCF-7 cells after 1 h; IC50 = 43 μM vs. P815 mastocytoma cells; IC50 = 23 μM vs. L1210 leukemia cells] and samples were sent to the National Cancer Institute for in-vitro screening (results included).

IT **413578-23-1P**, 2-(4-Benzyloxy-2-nitronaphthalen-1-yl)ethyl acetate
(preparation and hydrogenation of; preparation of achiral seco analogs of CC-1065 and the duocarmycins and compns. thereof for use in cancer therapy)

RN 413578-23-1 HCAPLUS

CN 1-Naphthaleneethanol, 2-nitro-4-(phenylmethoxy)-, acetate (ester) (9CI) (CA INDEX NAME)



IC ICM A61K031-44

ICS A61K031-4178; A61K031-4045; A61K031-401; A61K031-165
INCL 514397000; 514419000; 514423000; 514350000; 514617000; 548504000; 548530000; 564180000; 564182000
CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 7, 63
IT 413577-97-6P 413578-18-4P 413578-23-1P,
2-(4-Benzyloxy-2-nitronaphthalen-1-yl)ethyl acetate
(preparation and hydrogenation of; preparation of achiral seco analogs of CC-1065 and the duocarmycins and compns. thereof for use in cancer therapy)
REData is temporarily unavailable.

L37 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:293619 HCAPLUS Full-text
DOCUMENT NUMBER: 136:325360
TITLE: Compositions of achiral analogs of CC-1065 and the duocarmycins and methods of the use as anticancer agents
INVENTOR(S): Lee, Moses
PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030894	A2	20020418	WO 2001-US29160	20010919
WO 2002030894	A3	20020620		
W: CN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1320522	A2	20030625	EP 2001-973146	20010919
EP 1320522	B1	20051123		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2004511466	T	20040415	JP 2002-534280	20010919
AT 310724	T	20051215	AT 2001-973146	20010919
ES 2254492	T3	20060616	ES 2001-1973146	20010919
PRIORITY APPLN. INFO.:			US 2000-666160 A2	20000919
			WO 2001-US29160 W	20010919

OTHER SOURCE(S): MARPAT 136:325360
ED Entered STN: 19 Apr 2002
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

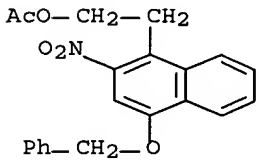
AB The present invention relates to novel achiral seco-analogs of the DNA minor groove and sequence-selective alkylating agents (+)-CC1065 and the duocarmycins, depicted as I, II, III, IV and V [X is a good leaving group, such as a Cl, Br, I, mesylate, tosylate, acetate, quaternary ammonium moiety, SH, alkylthio, alkylsulfoxyl, alkylsulfonyl; R = CH2Ph, CO2CH2Ph, H, CO2CH2C6H4NO2-4, N'-methylpiperazinyl-N-carbonyl; R1 is suitable minor groove

binding agent (such as the binding units of adozelesin and duocarmycins, netropsin and bisbenzimide) to enhance the interactions of the achiral seco-cyclopropaneindole (CI) or an achiral seco-duocarmycin with specific sequences of DNA, t-butoxy, benzyloxy, 9-flurenylmethyloxy or other common protecting groups for amines; R2, R3 = H, (un)branched C1-5-alkyl, Et, Pr, Bu, pentyl, hexyl; R4, R5 = H, short alkyl, CF3, alkyloxycarbonyl, CO2Me]. Thus, I (R = H, R1 = 5,6,7- trimethoxyindole) was prepared from [4-(benzyloxy)-2-nitrophenyl]ethyl chloride via regioselective hydrogenation with H2/PtO2 in THF, N-acylation with 5,6,7-trimethoxyindole-2-carboxylic acid in CH2Cl2 containing PyBOP and EtN(CHMe2)2, followed by hydrogenolysis with H2/Pd-C in THF containing HCO2NH4. The present invention is further directed to pharmaceutical compns. thereof, and as a method for treatment of cancer using the subject compds. Bioactivity of I (R = H, R1 = 5,6,7-trimethoxyindole) was determined [IC50 = 0.37 μM vs. K562 cells; IC50 = 0.94 μM vs. PC3 cells; IC50 = 1.5 μM vs. L1210 cells; 51±3 % form I DNA alkylation and 49±4% form II DNA alkylation at 0.1 mM; gel scans in Taq polymerase stop assay are given].

IT 413578-23-1P, 2-[4-Benzyloxy-2-nitronaphthalen-1-yl]ethyl acetate
(preparation of achiral analogs of CC-1065 and the duocarmycins as anticancer agents)

RN 413578-23-1 HCAPLUS

CN 1-Naphthaleneethanol, 2-nitro-4-(phenylmethoxy)-, acetate (ester) (9CI) (CA INDEX NAME)



IC ICM C07D209-00

CC 26-6 (Biomolecules and Their Synthetic Analogs)

IT 6860-79-3P, 2-(4-Benzyloxy-2-nitrophenyl)acetic acid 22907-68-2P, Methyl 3,4-Dinitrobenzoate 36692-49-6P, Methyl 3,4-Diaminobenzoate 118534-36-4P, 2-Benzyloxy-5-chloro-4-nitroaniline 157116-52-4P 157116-53-5P 413577-21-6P, 2-(4-Benzyloxy-2-nitrophenyl)ethanol 413577-22-7P, 2-(4-Benzyloxy-2-nitrophenyl)ethyl chloride 413577-23-8P, 2-(4-Benzyloxy-2-nitrophenyl)ethyl bromide 413577-24-9P, 2-(2-Amino-4-hydroxyphenyl)ethyl chloride 413577-25-0P, 2-(2-Amino-4-hydroxyphenyl)ethyl bromide 413577-26-1P, 2-(2-Amino-4-benzyloxyphenyl)ethyl chloride 413577-28-3P 413577-33-0P 413577-35-2P 413577-36-3P 413577-37-4P 413577-39-6P 413577-40-9P 413577-41-0P 413577-42-1P 413577-45-4P, N-(Benzyloxycarbonyl)-4-chloro-3-nitroaniline 413577-46-5P 413577-47-6P, 2-[4-{(Benzyloxycarbonyl)amino}-2-nitrophenyl]ethanol 413577-48-7P, 2-[4-{(Benzyloxycarbonyl)amino}-2-nitrophenyl]ethyl chloride 413577-49-8P, 2-[2-Amino-4-{(Nitrobenzyloxycarbonyl)amino}-phenyl]ethyl chloride 413577-50-1P 413577-51-2P 413577-52-3P 413577-53-4P, 2-(5-Amino-4-benzyloxy-2-nitrophenyl)acetic acid 413577-54-5P, 2-(5-Amino-4-benzyloxy-2-nitrophenyl)ethanol 413577-55-6P 413577-56-7P 413577-57-8P 413577-59-0P 413577-60-3P 413577-61-4P 413577-63-6P 413577-65-8P 413577-67-0P, Ethyl (2,4-dinitronaphthalen-1-yl)acetate 413577-69-2P, Ethyl (4-amino-2-nitronaphthalen-1-yl)acetate

413577-71-6P 413577-73-8P 413577-75-0P 413577-77-2P
413577-79-4P 413577-90-9P 413577-91-0P 413577-92-1P
413577-93-2P 413577-96-5P, 2-[4-Amino-2-nitronaphthalen-1-yl]ethyl acetate 413577-97-6P 413577-98-7P 413577-99-8P 413578-01-5P
413578-02-6P 413578-03-7P 413578-04-8P 413578-05-9P
413578-06-0P 413578-07-1P 413578-10-6P 413578-11-7P
413578-12-8P 413578-13-9P 413578-15-1P 413578-16-2P
413578-17-3P 413578-20-8P, Ethyl 2-[4-hydroxy-2-nitronaphthalen-1-yl]acetate 413578-21-9P, Ethyl 2-[4-benzyloxy-2-nitronaphthalen-1-yl]acetate 413578-22-0P, 2-[4-Benzyloxy-2-nitronaphthalen-1-yl]ethanol 413578-23-1P, 2-[4-Benzyloxy-2-nitronaphthalen-1-yl]ethyl acetate 413578-24-2P, 2-[2-Amino-4-benzyloxynaphthalen-1-yl]ethyl acetate 413578-25-3P 413578-26-4P 413578-27-5P
413578-28-6P 413578-29-7P
(preparation of achiral analogs of CC-1065 and the duocarmycins as anticancer agents)

REData is temporarily unavailable.

L37 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:275956 HCAPLUS Full-text
DOCUMENT NUMBER: 136:294655
TITLE: Aminopyridinyl-, aminoguanidinyl- and alkoxyguanidinyl- substituted phenyl acetamides as protease inhibitors
INVENTOR(S): Pan, Wenxi; Lu, Tianbao; Markotan, Thomas P.; Tomczuk, Bruce E.
PATENT ASSIGNEE(S): 3-Dimensional Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028825	A2	20020411	WO 2001-US31249	20011005
WO 2002028825	A3	20020613		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2423883	A1	20020411	CA 2001-2423883	20011005
AU 200211464	A	20020415	AU 2002-11464	20011005
US 2002061872	A1	20020523	US 2001-971000	20011005
US 6521663	B2	20030218		
EP 1324981	A2	20030709	EP 2001-979513	20011005
EP 1324981	B1	20060823		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200303149	A2	20040128	HU 2003-3149	20011005
BR 2001014263	A	20040302	BR 2001-14263	20011005
JP 2004510759	T	20040408	JP 2002-532411	20011005
ZA 2003003091	A	20040722	ZA 2003-3091	20011005

NZ 525438	A	20040924	NZ 2001-525438		20011005
CN 1568307	A	20050119	CN 2001-818254		20011005
AT 337299	T	20060915	AT 2001-979513		20011005
US 2003073833	A1	20030417	US 2002-262871		20021003
US 6900231	B2	20050531			
NO 2003001390	A	20030603	NO 2003-1390		20030326
IN 2003KN00504	A	20050311	IN 2003-KN504		20030423
US 2005159457	A1	20050721	US 2005-32297		20050110
PRIORITY APPLN. INFO.:			US 2000-238132P	P	20001006
			US 2001-971000	A3	20011005
			WO 2001-US31249	W	20011005
			US 2002-262871	A1	20021003

OTHER SOURCE(S): MARPAT 136:294655

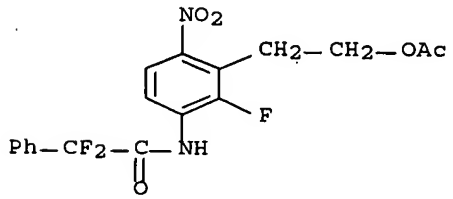
ED Entered STN: 12 Apr 2002

AB The compds. of the invention are potent inhibitors of proteases, especially trypsin-like serine proteases, such as thrombin and factor Xa. Compns. for inhibiting loss of blood platelets, inhibiting formation of blood platelet aggregates, inhibiting formation of fibrin, inhibiting thrombus formation, and inhibiting embolus formation are described. Other uses of compds. of the invention are as anticoagulants either embedded in or phys. linked to materials used in the manufacture of devices used in blood collection, blood circulation, and blood storage, such as catheters, blood dialysis machines, blood collection syringes and tubes, blood lines and stents. Addnl., the compds. can be detectably labeled and employed for in vivo imaging for thrombi. The 11 title compds. prepared have Ki values for human thrombin of between 0.0028 and 20μM. Among the 11 title compds. prepared by standard methods were 98% N-[2-(amidinoaminooxy)ethyl]-2-{3- [(2,2-difluoro-2-phenylethyl)amino]-6-chloro-2-fluorophenyl}acetamide, 99% N-[2-(amidinoaminooxy)ethyl]-2-{3-[2,2-difluoro-2-(4- fluoronaphthyl)ethylamino]-6-chloro-2-fluorophenyl}acetamide and 100% N-[2-(guanidinooxy)ethyl]-2-[2-chloro-5-(benzylsulfonylamino)phenyl]ac etamide.

IT **409081-72-7P 409081-87-4P**
(preparation of aminopyridinyl-, aminoguanidinyl- and alkoxyguanidinyl-substituted phenylacetamides as anticoagulants)

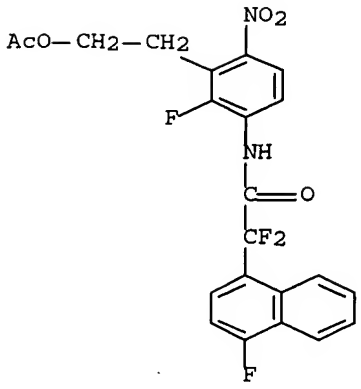
RN 409081-72-7 HCAPLUS

CN Benzeneacetamide, N-[3-[2-(acetyloxy)ethyl]-2-fluoro-4-nitrophenyl]-α,α-difluoro- (9CI) (CA INDEX NAME)



RN 409081-87-4 HCAPLUS

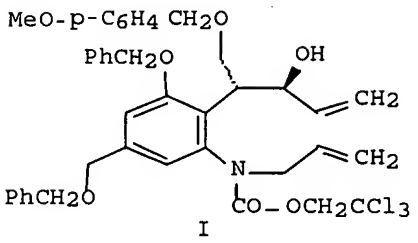
CN 1-Naphthaleneacetamide, N-[3-[2-(acetyloxy)ethyl]-2-fluoro-4-nitrophenyl]-α,α,4-trifluoro- (9CI) (CA INDEX NAME)



IC ICM C07C279-00
ICS C07D213-40; A61K031-155; A61K031-44
CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 7
IT 312-24-3P, 2,2-Difluoro-2-phenylacetyl chloride 360-03-2P, 2,2-Difluoro-2-phenylacetic acid 2248-46-6P, Ethyl 2,2-difluoro-2-phenylacetate 19281-12-0P 22474-47-1P, 2-Methyl-5-nitrobenzyl alcohol 37777-70-1P, 2-Chloro-5-nitrophenylacetic acid 100278-66-8P 100278-67-9P, 2-Allyl-3-methyl-6-nitrophenol 141428-47-9P 141449-03-8P 141449-04-9P 141449-81-2P 225096-22-0P 287119-83-9P, 2-Methyl-5-nitrophenylacetic acid 409081-71-6P **409081-72-7P** 409081-73-8P 409081-74-9P 409081-75-0P 409081-76-1P 409081-77-2P 409081-78-3P 409081-79-4P 409081-81-8P 409081-82-9P 409081-83-0P 409081-84-1P 409081-85-2P 409081-86-3P **409081-87-4P** 409081-88-5P 409081-89-6P 409081-90-9P 409081-91-0P 409081-92-1P 409081-93-2P 409081-94-3P 409081-95-4P 409081-96-5P 409081-97-6P 409081-98-7P 409081-99-8P 409082-00-4P 409082-01-5P, Ethyl 2-chloro-5-nitrophenylacetate 409082-02-6P, Ethyl 5-amino-2-chlorophenylacetate 409082-04-8P 409082-06-0P 409082-08-2P 409082-10-6P, 2-Methyl-5-nitrobenzyl methanesulfonate 409082-11-7P, 2-Methyl-5-nitrophenylacetonitrile 409082-15-1P 409082-17-3P 409082-19-5P 409082-21-9P 409082-22-0P 409082-23-1P 409082-24-2P 409082-25-3P 409082-26-4P 409082-27-5P 409082-28-6P 409082-29-7P 409082-30-0P 409082-31-1P 409082-32-2P 409082-33-3P 409082-34-4P 409082-35-5P 409082-36-6P
(preparation of aminopyridinyl-, aminoguanidinyl- and alkoxyguanidinyl-substituted phenylacetamides as anticoagulants)
REData is temporarily unavailable.

L37 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:746410 HCAPLUS Full-text
DOCUMENT NUMBER: 134:42002
TITLE: Application of ring-closing metathesis to the formal total synthesis of (+)-FR900482
AUTHOR(S): Fellows, Ingrid M.; Kaelin, David E., Jr.; Martin, Stephen F.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712, USA

SOURCE: Journal of the American Chemical Society (2000), 122(44), 10781-10787
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:42002
ED Entered STN: 24 Oct 2000
GI



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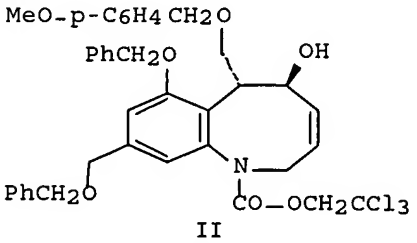

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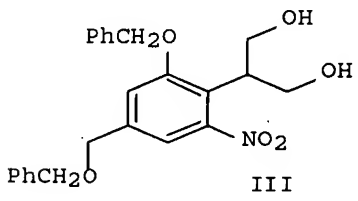
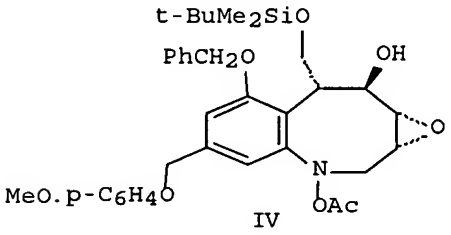


III



IV

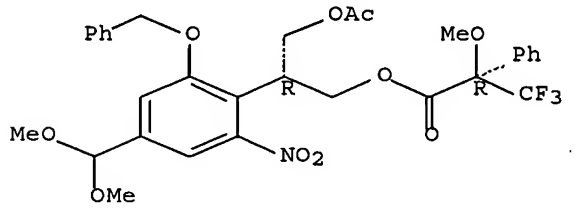
AB A formal, enantioselective synthesis of the antitumor antibiotic (+)-FR900482 has been completed using an approach that featured the ring-closing metathesis of the diene I to give the key intermediate benzazocine II. Although several initial protecting-group strategies unexpectedly failed at various stages of the endeavor, the successful approach to FR900482 involved the conversion of com. available 5-nitrovanillin into the prochiral diol III. The manipulations of the residues on the aromatic ring of 5-nitrovanillin were straightforward, and the diol array in III was introduced by the hydride reduction of a malonate, which was in turn prepared by a nucleophilic substitution of a triflate. Adjustment of alc.-protecting groups and refunctionalization of the aromatic nitro group led to the protected N-allylamine. Elaboration of the diol array via a highly stereoselective Grignard addition furnished the diene I. Ring-closing metathesis of I using the Grubbs catalyst cleanly afforded the benzazocine II. A tactic originally conceived for preparing an aziridine derivative by introduction of the aziridine ring onto II was impractical because the iodo cyclization of the allylic tosylcarbamate was neither efficient nor selective. Hence, II was transformed into IV, which was a key intermediate in Fukuyama's elegant synthesis of racemic FR900482, thereby completing a formal synthesis of the alkaloid. The prochiral diol III was enzymically desymmetrized using Pseudomonas species lipase to give the (S)-acetate in 94% enantiomeric excess. Inasmuch as subsequent adjustment of the alc.-protecting groups gave the protected intermediate of III in enantiomerically pure form, an enantioselective synthesis of (+)-FR900482 has also been completed in a formal sense.
IT 312732-09-5P

(crystal structure; formal total synthesis of (+)-FR900482 via ring-closing metathesis)

RN 312732-09-5 HCAPLUS

CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R)-3-(acetyloxy)-2-[4-(dimethoxymethyl)-2-nitro-6-(phenylmethoxy)phenyl]propyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

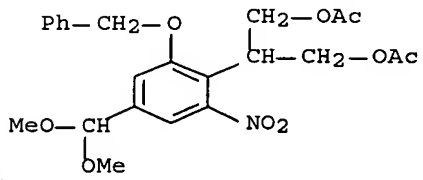


IT 312732-07-3P

(formal total synthesis of (+)-FR900482 via ring-closing metathesis)

RN 312732-07-3 HCAPLUS

CN 1,3-Propanediol, 2-[4-(dimethoxymethyl)-2-nitro-6-(phenylmethoxy)phenyl]-, diacetate (ester) (9CI) (CA INDEX NAME)



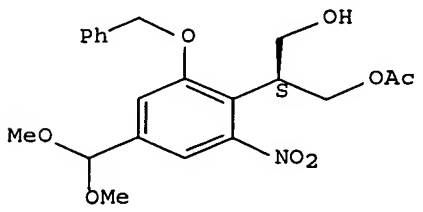
IT 312731-74-1P 312731-83-2P

(formal total synthesis of (+)-FR900482 via ring-closing metathesis)

RN 312731-74-1 HCAPLUS

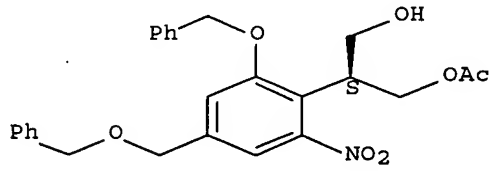
CN 1,3-Propanediol, 2-[4-(dimethoxymethyl)-2-nitro-6-(phenylmethoxy)phenyl]-, monoacetate (ester), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



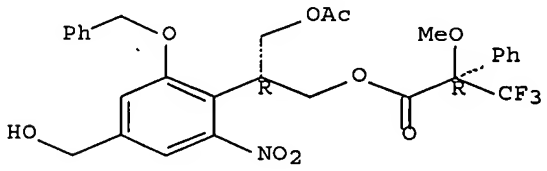
RN 312731-83-2 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-6-(phenylmethoxy)-4-[(phenylmethoxy)methyl]phenyl]-, monoacetate (ester), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



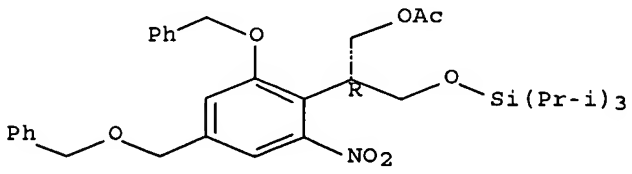
IT 312732-12-0P 312732-15-3P 312732-24-4P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
RN 312732-12-0 HCAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R)-3-(acetyloxy)-2-[4-(hydroxymethyl)-2-nitro-6-(phenylmethoxy)phenyl]propyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312732-15-3 HCAPLUS
CN Benzeneethanol, 2-nitro-6-(phenylmethoxy)-4-[(phenylmethoxy)methyl]-β-[[[tris(1-methylethyl)silyl]oxy]methyl]-, acetate (ester), (βR)- (9CI) (CA INDEX NAME)

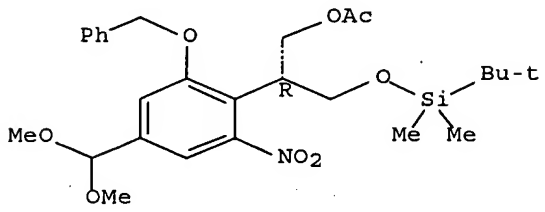
Absolute stereochemistry. Rotation (-).



RN 312732-24-4 HCAPLUS
CN Benzeneethanol, 4-(dimethoxymethyl)-β-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-nitro-6-(phenylmethoxy)-,

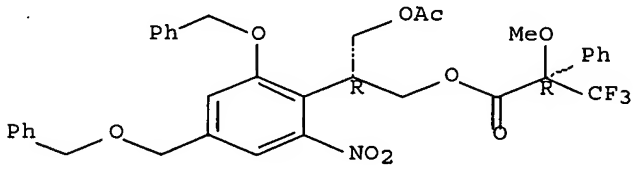
acetate (ester), (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



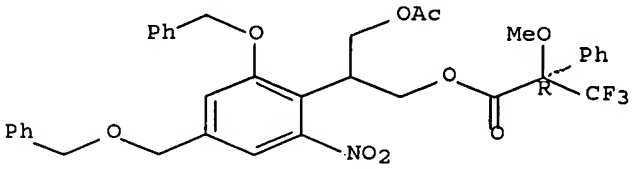
IT 312732-13-1P 312732-14-2P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
RN 312732-13-1 HCAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R)-3-(acetyloxy)-2-[2-nitro-6-(phenylmethoxy)-4-[(phenylmethoxy)methyl]phenyl]propyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312732-14-2 HCAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 3-(acetyloxy)-2-[2-nitro-6-(phenylmethoxy)-4-[(phenylmethoxy)methyl]phenyl]propyl ester, (αR)- (9CI) (CA INDEX NAME)

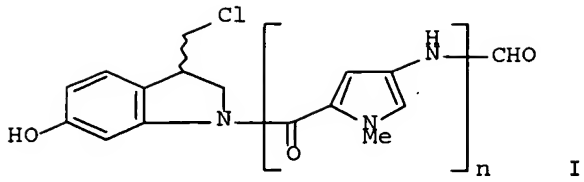
Absolute stereochemistry.



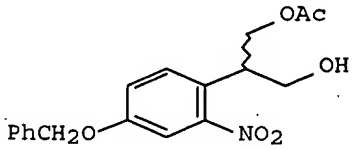
CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 75
IT 312731-97-8P 312732-09-5P
(crystal structure; formal total synthesis of (+)-FR900482 via

ring-closing metathesis)
IT 312732-07-3P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
IT 312731-74-1P 312731-83-2P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
IT 116313-85-0P 312327-13-2P 312731-69-4P 312731-70-7P
312731-71-8P 312731-72-9P 312731-73-0P 312731-76-3P
312731-77-4P 312731-78-5P 312731-79-6P 312731-81-0P
312731-82-1P 312731-85-4P 312731-86-5P 312731-87-6P
312731-88-7P 312731-89-8P 312731-92-3P 312731-93-4P
312731-94-5P 312731-95-6P 312731-99-0P 312732-00-6P
312732-01-7P 312732-02-8P 312732-03-9P 312732-08-4P
312732-10-8P 312732-11-9P 312732-12-0P
312732-15-3P 312732-16-4P 312732-17-5P 312732-18-6P
312732-19-7P 312732-20-0P 312732-21-1P 312732-22-2P
312732-23-3P 312732-24-4P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
IT 312731-75-2P 312731-80-9P 312731-84-3P 312731-91-2P
312732-04-0P 312732-13-1P 312732-14-2P
(formal total synthesis of (+)-FR900482 via ring-closing metathesis)
REData is temporarily unavailable.

L37 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:721722 HCAPLUS Full-text
DOCUMENT NUMBER: 128:22780
TITLE: Synthesis and evaluation of the hybrid molecules possessing DNA-cleaving activity
AUTHOR(S): Shishido, Kozo; Haruna, Shigenori; Yamamura, Chisato; Iitsuka, Hiromi; Nemoto, Hisao; Shinohara, Yasuo; Shibuya, Masayuki
CORPORATE SOURCE: Institute for Medicinal Resources, University of Tokushima, Sho, 770, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(20), 2617-2622
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 17 Nov 1997
GI



I



II

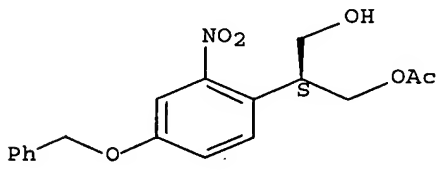
AB The design and synthesis of enantiomerically enriched hybrid mols., (S)- and (R)-indolines I (n = 1-3), have been accomplished by employing the lipase-mediated asym. acetylation of prochiral diol II as the key step. Evaluation of their DNA-cleaving activity has revealed the unnatural type of enantiomer (R)-I to be more potent than (S)-I with natural configuration.

IT 184046-60-4P 184046-61-5P
(preparation and DNA-cleaving activity of indolines)

RN 184046-60-4 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (S)- (9CI) (CA INDEX NAME)

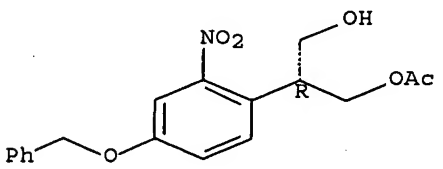
Absolute stereochemistry. Rotation (-).



RN 184046-61-5 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

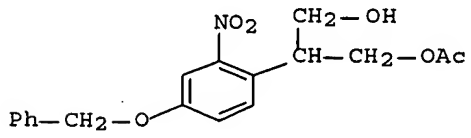


CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

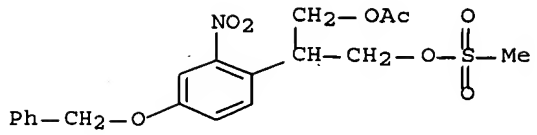
IT 183853-90-9P 183853-91-0P 183853-92-1P 183853-93-2P

183853-94-3P 183858-76-6P **184046-60-4P**
184046-61-5P 184046-62-6P 184046-63-7P
(preparation and DNA-cleaving activity of indolines)
REData is temporarily unavailable.

L37 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:403816 HCAPLUS Full-text
DOCUMENT NUMBER: 127:130541
TITLE: Synthesis, DNA binding and cytotoxicity of 1-[[ω-(9-acridinyl)amino]alkyl]carbonyl-3-(chloromethyl)-6-hydroxyindolines, a new class of DNA-target alkylating agents
AUTHOR(S): Fan, Jun-Yao; Tercel, Moana; Denny, William A.
CORPORATE SOURCE: Cancer Society Research Laboratory, Faculty of Medicine and Health Sciences, The University of Auckland, Auckland, N. Z.
SOURCE: Anti-Cancer Drug Design (1997), 12(4), 277-293
CODEN: ACDDEA; ISSN: 0266-9536
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 30 Jun 1997
AB We report the first synthesis of examples of the seco-CI DNA alkylating moiety 3-(chloromethyl)-6-hydroxyindoline linked to a 9-aminoacridine DNA-intercalating units. The sequence-specificity of DNA alkylation by these compds. was studied by the gel electrophoresis cleavage assay. In contrast to the known trimethoxyindole-linked compound, which alkylates exclusively at N3 of adenines in the minor groove, the acridine-linked analogs alkylate predominantly at the N7 of guanines in the major groove (the first CI analogs reported to do so), although DNase I footprinting expts. show that the initial non-covalent binding of the acridine-linked analogs is not base sequence selective. DNA unwinding expts. show that the acridine moiety of the acridine-linked analogs remains intercalated after alkylation.
IT **157485-05-7P 157485-06-8P**
(DNA binding, cytotoxicity, and synthesis of 1-[[ω-(9-acridinyl)amino]alkyl]carbonyl-3-(chloromethyl)-6-hydroxyindolines)
RN 157485-05-7 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester) (9CI) (CA INDEX NAME)



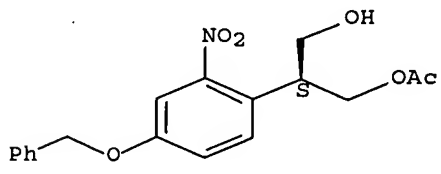
RN 157485-06-8 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, acetate (ester) methanesulfonate (ester) (9CI) (CA INDEX NAME)



CC 1-6 (Pharmacology)
IT 106014-83-9P 106014-84-0P 119880-00-1P 119880-03-4P
119880-05-6P 151384-87-1P 153081-78-8P 157485-05-7P
157485-06-8P 193078-55-6P 193078-58-9P 193078-59-0P
193078-60-3P
(DNA binding, cytotoxicity, and synthesis of 1-[[ω-(9-acridinyl)amino]alkyl]carbonyl-3-(chloromethyl)-6-hydroxyindolines)
REData is temporarily unavailable.

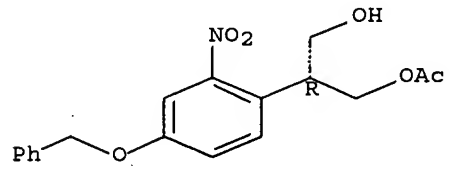
L37 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:45375 HCAPLUS Full-text
DOCUMENT NUMBER: 126:117812
TITLE: Enzymic preparation of an optically active precursor of the CC-1065/duocarmycin pharmacophore
AUTHOR(S): Chenevert, Robert; Courchesne, Gabriel
CORPORATE SOURCE: Departement de Chimie, Faculte des Sciences et de Genie, Universite Laval, QC, G1K 7P4, Can.
SOURCE: Chemistry Letters (1997), (1), 11-12
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:117812
ED Entered STN: 22 Jan 1997
AB Acetylation of 2-[4-(benzyloxy)-2-nitrophenyl]propane-1,3-diol with vinyl acetate in the presence of porcine pancreatic lipase gave the (R)-monoacetate (ee-92%). The (S)-mono-acetate was obtained via acetylation of the diol followed by transesterification in ethanol in the presence of the same enzyme. Incorporation of these optically active mono-acetates into the established synthetic routes provided access to both enantiomers of the common pharmacophore of CC-1065/duocarmycin.
IT 184046-60-4P
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
RN 184046-60-4 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



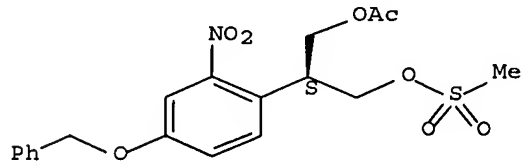
IT **184046-61-5P**
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
RN 184046-61-5 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

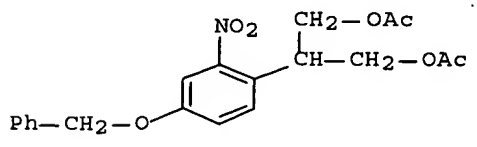


IT **186144-33-2P**
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
RN 186144-33-2 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, acetate (ester) methanesulfonate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **186144-29-6P**
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
RN 186144-29-6 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

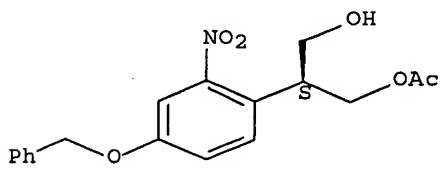


CC 26-6 (Biomolecules and Their Synthetic Analogs)
IT **184046-60-4P**
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)

IT 184046-61-5P
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
IT 128049-46-7P 128049-48-9P 128049-50-3P 186144-33-2P
186144-35-4P
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
IT 186144-29-6P
(enzymic preparation of CC-1065/duocarmycin pharmacophore precursor, cyclopropaindolone)
REData is temporarily unavailable.

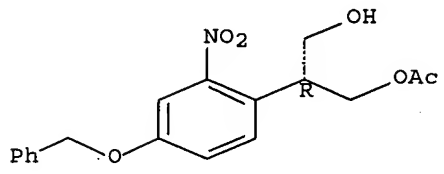
L37 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:703770 HCAPLUS Full-text
DOCUMENT NUMBER: 126:3234
TITLE: Development of the molecules possessing DNA cleaving activity
AUTHOR(S): Haruna, Shigenori; Irie, Osamu; Shishido, Kozo; Iitsuka, Hiromi; Nemoto, Hisao; Shibuya, Masayuki
CORPORATE SOURCE: Institute Medicinal Resources, University Tokushima, Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1996), 38th, 745-750
CODEN: TYKYDS
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
ED Entered STN: 27 Nov 1996
AB Fourteen mols., which contain the alkylating subunit of duocarmycins, CC-1065, and azinomycins linked by a pyrrole amide moiety of distamycin A, were chemical synthesized and their DNA cleaving activity determined Computer modeling was used to study their interaction with DNA. The DNA cleaving activities depended on the absolute structure of the compds. and the length of the pyrrole amide moiety. A compound recognized specifically the A-T rich regions and the alkylation occurred at adenine bases. The distance between adenine N-3 and the alkylating carbon was crucial in the reaction.
IT 184046-60-4P 184046-61-5P
(in DNA cleaving agent preparation; DNA cleaving activity of synthetic compds. containing alkylating subunits of duocarmycins and azinomycins)
RN 184046-60-4 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



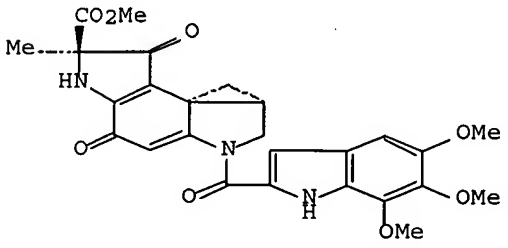
RN 184046-61-5 HCAPLUS
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

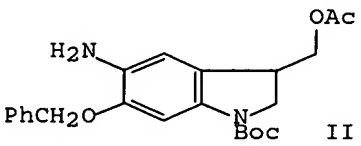


CC 6-2 (General Biochemistry)
Section cross-reference(s): 3
IT 22250-90-4P 77716-14-4P 77716-18-8P 77716-19-9P 77716-21-3P
106014-83-9P 106319-56-6P 106400-07-1P 120122-47-6P
127661-27-2P 183853-88-5P 183853-89-6P 183853-90-9P
183853-91-0P 183853-92-1P 183853-93-2P 183853-94-3P
183853-95-4P 183853-96-5P 183853-97-6P 183858-76-6P
184046-60-4P 184046-61-5P 184046-62-6P
184046-63-7P
(in DNA cleaving agent preparation; DNA cleaving activity of synthetic compds. containing alkylating subunits of duocarmycins and azinomycins)
REData is temporarily unavailable.

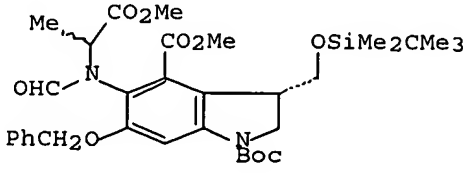
L37 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:557347 HCAPLUS Full-text
DOCUMENT NUMBER: 121:157347
TITLE: Synthetic studies on duocarmycin. 1. Total synthesis of dL-duocarmycin A and its 2-epimer
AUTHOR(S): Fukuda, Yasumichi; Itoh, Yoshio; Nakatani, Kazuhiko; Terashima, Shiro
CORPORATE SOURCE: Sagami Chem. Res. Cent., Kanagawa, 229, Japan
SOURCE: Tetrahedron (1994), 50(9), 2793-808
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:157347
ED Entered STN: 01 Oct 1994
GI



I



II



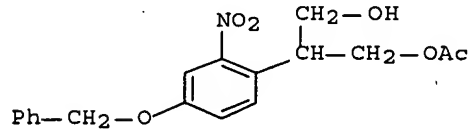
III

AB The title synthesis of dL-duocarmycin A (I) and its 2-epimer was first achieved by employing novel methoxycarbonylation of the C4-position of the 5-aminoindoline II by way of the isatin and subsequent Dieckmann cyclization of indolecarboxylate III to the Me 2-methylindoxyl-2- carboxylate as key steps. In vitro cytotoxicity assay against P388 murine leukemia obviously disclosed that cytotoxicities of the synthesized compds. are comparable and almost half of that of natural (+)-duocarmycin A.

IT **157485-05-7P**
(preparation and mesylation of)

RN 157485-05-7 HCAPLUS

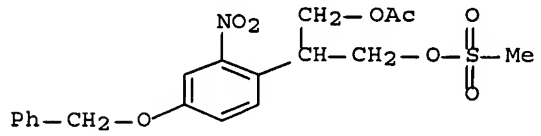
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester) (9CI) (CA INDEX NAME)



IT **157485-06-8P**
(preparation, reduction-cyclization, and protection of)

RN 157485-06-8 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, acetate (ester) methanesulfonate (ester) (9CI) (CA INDEX NAME)



CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT **157485-05-7P** 157485-10-4P 157485-11-5P
(preparation and mesylation of)

IT **157485-06-8P**
(preparation, reduction-cyclization, and protection of)

REData is temporarily unavailable.

L37 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:299294 HCAPLUS Full-text

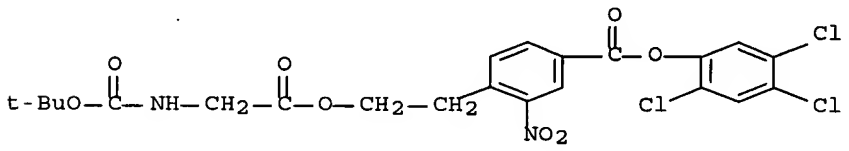
DOCUMENT NUMBER: 120:299294

TITLE: Stepwise Solid-Phase Synthesis of the Nucleopeptide Phac-Phe-Val-Ser(p3'ACT)-Gly-OH

AUTHOR(S): Robles, Jordi; Pedroso, Enrique; Grandas, Anna

CORPORATE SOURCE: Facultat de Quimica, Universitat de Barcelona, Barcelona, E-08028, Spain

SOURCE: Journal of Organic Chemistry (1994), 59(9), 2482-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 11 Jun 1994
AB The nucleopeptide Phac-Phe-Val-Ser(p3'ACT)-Gly-OH (Phac = PhCH2CO) with a phosphodiester bond between the side chain hydroxyl group of a serine residue and the 3' end of a trinucleotide, has been synthesized by a stepwise procedure. The peptide was first assembled on an insol. matrix and the oligonucleotide chain elongation was then carried out at the serine hydroxyl group of the resin-linked peptide by the phosphite triester approach using standard phosphoramidite derivs. Mild basic conditions were used for the final deprotection of the permanent protecting groups.
IT **155211-21-5P**
(preparation and solid-phase coupling reactions of, in preparation of nucleopeptide)
RN 155211-21-5 HCAPLUS
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, 2-[2-nitro-4-[(2,4,5-trichlorophenoxy)carbonyl]phenyl]ethyl ester (9CI) (CA INDEX NAME)



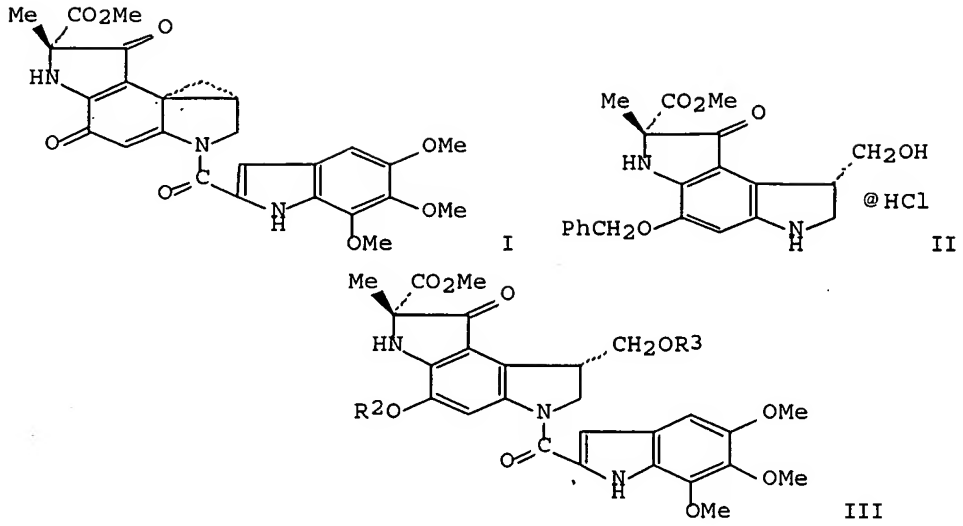
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 33
IT **155211-21-5P** 155211-22-6DP, amide with (aminomethyl)polystyrene
(preparation and solid-phase coupling reactions of, in preparation of nucleopeptide)
REData is temporarily unavailable.

L37 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:591589 HCAPLUS Full-text
DOCUMENT NUMBER: 117:191589
TITLE: Preparation of 2-epiduocarmycin A as antitumor agent
INVENTOR(S): Terajima, Atsuro; Fukuda, Yasumichi; Nakatani, Kazuhiko; Ito, Yoshio
PATENT ASSIGNEE(S): Zaidan Hojin Sagami Chuo Kagaku Kenkyusho, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04099774	A	19920331	JP 1990-213741	19900814
PRIORITY APPLN. INFO.:			JP 1990-213741	19900814

OTHER SOURCE(S): MARPAT 117:191589
ED Entered STN: 15 Nov 1992

GI

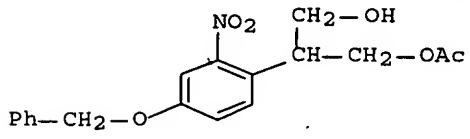


AB 2-Epiduocarmycin A (I) and its intermediates are prepared Condensation of (2S,8S)-II with 6,7,8-trimethoxy-1H-indole-2-carboxylic acid and 1-(3-dimethylaminopropyl)ethylcarbodiimide HCl in DMF gave 62% indolyl derivative (2S,8S)-III (R2 = PhCH2, R3 = H), which was mesylated with MeSO2Cl in CH2Cl2 to give 99% mesylate (2S,8S)-III (R2 = PhCH2, R3 = MeSO2) (IV). Hydrogenolysis of IV over 10% Pd-C gave 83% phenolic derivative (2S,8S)-III (R2 = H, R3 = MeSO2), which was treated with NaH (50% oil dispersion) in THF with stirring at room temperature to give 56% (DL)-I, which showed IC50 of 1.7 + 10-4 μg/mL against P-388 leukemic cells.

IT **157485-05-7P 157485-06-8P**
(preparation and reaction of, in preparation of antitumor agent)

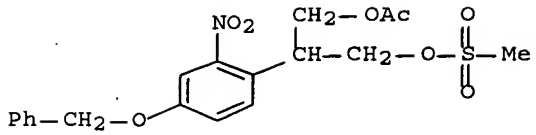
RN 157485-05-7 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester) (9CI) (CA INDEX NAME)



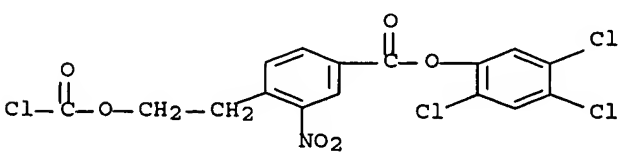
RN 157485-06-8 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, acetate (ester) methanesulfonate (ester) (9CI) (CA INDEX NAME)



IC ICM C07D487-04
ICA A61K031-40
ICI C07D487-04, C07D207-00, C07D209-00
CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
IT 118292-37-8P 128781-06-6P 128781-07-7P 132436-57-8P
132628-58-1P 132628-59-2P 132628-60-5P 132628-62-7P
132628-63-8P 132628-64-9P 132628-65-0P 132628-66-1P
132628-67-2P 132628-68-3P 132628-69-4P 132628-70-7P
132628-71-8P 132628-72-9P 132628-74-1P 132628-75-2P
143314-85-6P 143314-86-7P 143314-87-8P 143314-88-9P
143874-46-8P **157485-05-7P 157485-06-8P**
(preparation and reaction of, in preparation of antitumor agent)
REData is temporarily unavailable.

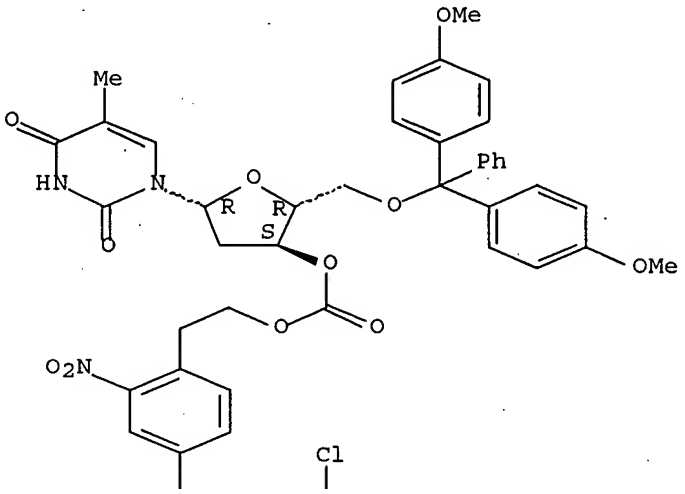
L37 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:470220 HCAPLUS Full-text
DOCUMENT NUMBER: 117:70220
TITLE: A synthetic procedure for the preparation of oligonucleotides without using ammonia and its application for the synthesis of oligonucleotides containing O-4-alkyl thymidines
AUTHOR(S): Eritja, Ramon; Robles, Jordi; Avino, Anna; Albericio, Fernando; Pedroso, Enrique
CORPORATE SOURCE: Dep. Mol. Genet., CSIC, Barcelona, 08034, Spain
SOURCE: Tetrahedron (1992), 48(20), 4171-82
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 23 Aug 1992
AB The preparation of 5'-O-dimethoxytrityl (DMT) and p-nitrophenylethyl (NPEOC, NPE) protected nucleosides linked to 4-(2-hydroxyethyl)-3- nitrobenzoic acid derivs. is described. These products attached to controlled-pore glass supports and together with DMT and NPE-protected nucleoside cyanoethyl phosphoramidites permits a first time preparation of short (6-13 bases) oligonucleotides containing the ammonia sensitive mutagenic bases O-4-Pr and O-4-Bu thymidines, 5' GCTprAGC 3' and 5' GCTbuAGC 3'.
IT **134403-92-2P**
(preparation and conversion to protected nucleosides)
RN 134403-92-2 HCAPLUS
CN Benzoic acid, 4-[2-[(chlorocarbonyl)oxy]ethyl]-3-nitro-, 2,4,5-trichlorophenyl ester (9CI) (CA INDEX NAME)



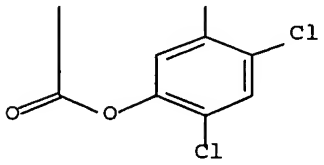
IT 134403-95-5P
(preparation of)
RN 134403-95-5 HCAPLUS
CN Thymidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-, 3'-[2-[2-nitro-4-[(2,4,5-trichlorophenoxy)carbonyl]phenyl]ethyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



CC 33-9 (Carbohydrates)
IT 134403-92-2P 134403-97-7P
(preparation and conversion to protected nucleosides)
IT 134403-93-3P 134403-94-4P 134403-95-5P 134403-98-8P
134403-99-9P 134425-73-3P 142599-79-9P 142599-80-2P
142599-81-3P 142599-82-4P 142599-83-5P 142599-84-6P
142617-31-0P
(preparation of)
REData is temporarily unavailable.

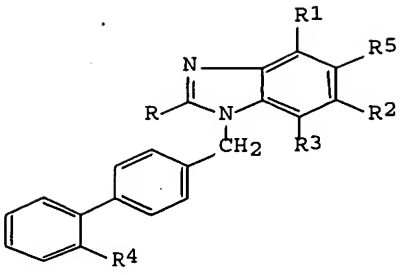
L37 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:151759 HCAPLUS Full-text

DOCUMENT NUMBER: 116:151759
TITLE: Benzimidazole derivatives, process and intermediates for their preparation, their use as medicaments (especially antihypertensives), and pharmaceutical compositions containing them
INVENTOR(S): Fortin, Michel; Frechet, Daniel; Hamon, Gilles; Jouquey, Simone; Vevert, Jean Paul
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 73 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 461039	A1	19911211	EP 1991-401480	19910606
EP 461039	B1	19980916		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2663028	A1	19911213	FR 1990-7135	19900608
FR 2663028	B1	19941014		
FR 2670489	A1	19920619	FR 1990-15811	19901218
FR 2670489	B1	19941014		
FR 2674523	A1	19921002	FR 1991-3778	19910328
AU 9178200	A	19911212	AU 1991-78200	19910606
AT 171177	T	19981015	AT 1991-401480	19910606
ES 2121773	T3	19981216	ES 1991-401480	19910606
CA 2044124	A1	19911209	CA 1991-2044124	19910607
AU 9178246	A	19911212	AU 1991-78246	19910607
AU 657478	B2	19950316		
HU 58061	A2	19920128	HU 1991-1914	19910607
JP 04235973	A	19920825	JP 1991-162300	19910607
JP 3084302	B2	20000904		
ZA 9104376	A	19920826	ZA 1991-4376	19910607
RU 2067095	C1	19960927	RU 1991-4895873	19910607
KR 204633	B1	19990615	KR 1991-9418	19910607
CN 1057256	A	19911225	CN 1991-103858	19910608
CN 1045771	B	19991020		

PRIORITY APPLN. INFO.: FR 1990-7135 A 19900608
FR 1990-15811 A 19901218
FR 1991-3778 A 19910328

OTHER SOURCE(S): MARPAT 116:151759
ED Entered STN: 17 Apr 1992
GI



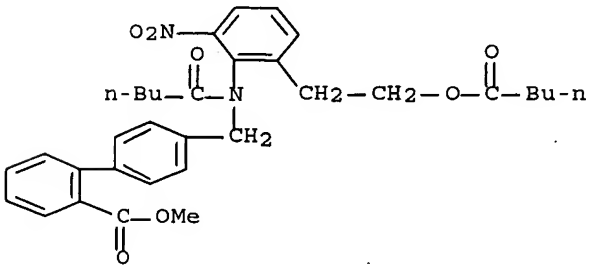
I

AB (Biphenylylmethyl)benzimidazoles I [R = alkyl, alkenyl; either (a) R1 = R2 = R3 = R5 = H; or (b) R2 or R5 = H, and other = H, CH2OR10, or certain amino groups; R1 or R3 = H, and other = OR6, CO2R7, or R11; or (c) ≤1 of R1, R2, R3, R5 = H, and others = CH2OR10, OR6, CO2R7, R11, or certain amino groups; R4 = CO2H or its esters or salts, tetrazolyl, (CH2)mSO2XR12; R6, R7, R10 = H, alkyl, alkenyl; R11 = alkenyl, acyl, (un)substituted alkyl, certain amino groups; m = 0-4; either XR12 = NH2, or X = bond, NH, NHCONH, NHCO and R12 = (un)substituted alkyl, alkenyl, or aryl] were prepared as antihypertensives, and also for use in other cardiac, renal, gastrointestinal, and gynecol. disorders. For example, Me 4'-[N-[2-(methoxycarbonyl)-6-nitrophenyl]-N-(pentanoyl)aminomethylbiphenyl-2-carboxylate (preparation given) underwent hydrogenation over Pd/C, cyclization of the resultant 6-amino analog by HCl in EtOAc-Me2CHOH, and saponification by NaOH in aqueous EtOH, to give I (R = Bu; R1 = R2 = R5 = H; R3 = R4 = CO2H) (II). The ID50 of II for antagonism of angiotensin II-induced pressive response in anesthetized, demedullated rats was 0.3 mg/kg. Two addnl. tests for angiotensin II antagonism, two formulations, and 23 more synthetic examples are given.

IT **139743-13-8P**
(preparation and reaction of, in preparation of benzimidazole antihypertensives)

RN 139743-13-8 HCAPLUS

CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[[2-nitro-6-[2-[(1-oxopentyl)oxy]ethyl]phenyl](1-oxopentyl)amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)



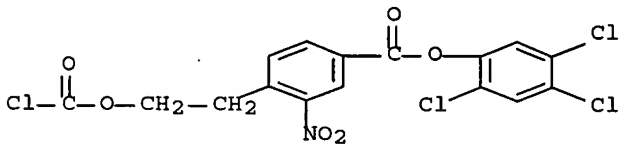
IC ICM C07D403-10
ICS C07D235-08; C07C229-38; C07D257-04; C07C233-54; C07C233-43; C07C233-40; C07C233-25; C07C233-15; A61K031-41

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 606-18-8P 57113-91-4P 59907-22-1P 90417-80-4P 136285-36-4P

139743-06-9P 139743-07-0P 139743-08-1P 139743-09-2P
139743-10-5P 139743-11-6P 139743-12-7P 139743-13-8P
139743-14-9P 139743-15-0P
(preparation and reaction of, in preparation of benzimidazole antihypertensives)
REData is temporarily unavailable.

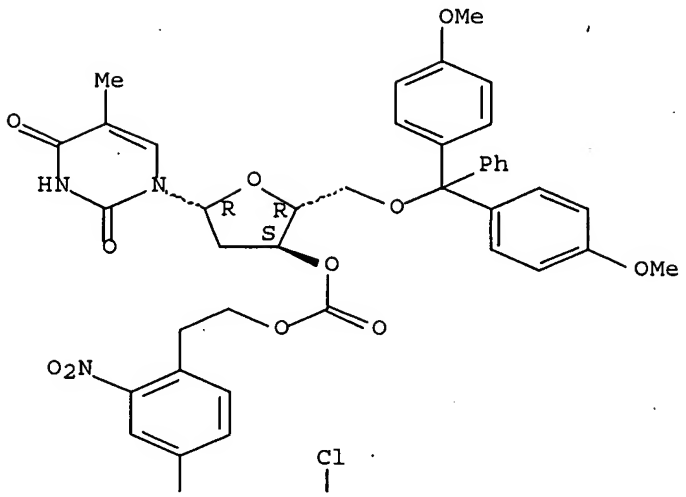
L37 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:429800 HCAPLUS Full-text
DOCUMENT NUMBER: 115:29800
TITLE: NPE-resin, a new approach to the solid-phase synthesis of protected peptides and oligonucleotides. I. Synthesis of the supports and their application to oligonucleotide synthesis
AUTHOR(S): Eritja, Ramon; Robles, Jordi; Fernandez-Forner, Dolors; Albericio, Fernando; Giralt, Ernest; Pedroso, Enrique
CORPORATE SOURCE: Dep. Mol. Genet., CSIC, Barcelona, E-08034, Spain
SOURCE: Tetrahedron Letters (1991), 32(11), 1511-14
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 27 Jul 1991
AB The preparation of polymeric supports containing a base labile 2-(2-nitrophenyl) Et linkage and the attachment of protected nucleosides is described together with their application to oligonucleotide synthesis.
IT 134403-92-2P
(preparation and reaction of, with thymidine derivative)
RN 134403-92-2 HCAPLUS
CN Benzoic acid, 4-[2-[(chlorocarbonyl)oxy]ethyl]-3-nitro-, 2,4,5-trichlorophenyl ester (9CI) (CA INDEX NAME)



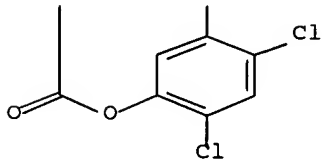
IT 134403-95-5P
(preparation of, in synthesis of oligonucleotides)
RN 134403-95-5 HCAPLUS
CN Thymidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-, 3'-[2-[2-nitro-4-[(2,4,5-trichlorophenoxy)carbonyl]phenyl]ethyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

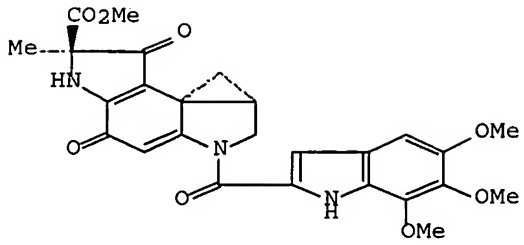


PAGE 2-A

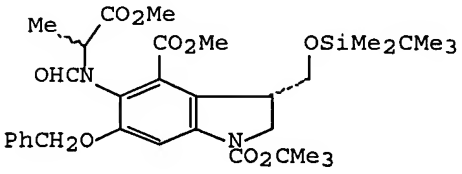


CC 33-9 (Carbohydrates)
Section cross-reference(s): 34
IT 134403-90-0DP, solid support 134403-92-2P 134403-97-7P
(preparation and reaction of, with thymidine derivative)
IT 134403-95-5P 134403-96-6DP, solid support
(preparation of, in synthesis of oligonucleotides)
REData is temporarily unavailable.

L37 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:142962 HCAPLUS Full-text
DOCUMENT NUMBER: 114:142962
TITLE: First total synthesis of dl-duocarmycin A
AUTHOR(S): Fukuda, Yasumichi; Nakatani, Kazuhiko; Ito, Yoshio; Terashima, Shiro
CORPORATE SOURCE: Sagami Chem. Res. Cent., Sagamihara, 229, Japan
SOURCE: Tetrahedron Letters (1990), 31(46), 6699-702
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:142962
ED Entered STN: 19 Apr 1991
GI



I



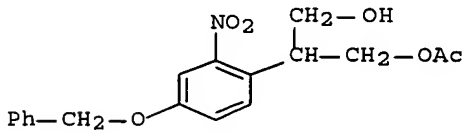
II

AB Synthesis of the title compound (I) was achieved by featuring introduction of a methoxycarbonyl group into the C-4 position of a 5-aminoindoline nucleus by way of an isatin derivative and subsequent ring closure to a Me 2-methylindoxyl-2-carboxylate system by the Dieckmann cyclization the indolylformamide II.

IT **157485-05-7P**
(preparation and mesylation of)

RN 157485-05-7 HCAPLUS

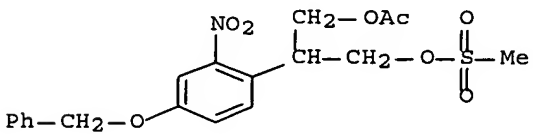
CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, monoacetate (ester) (9CI) (CA INDEX NAME)



IT **157485-06-8P**
(preparation and reductive cyclization of)

RN 157485-06-8 HCAPLUS

CN 1,3-Propanediol, 2-[2-nitro-4-(phenylmethoxy)phenyl]-, acetate (ester) methanesulfonate (ester) (9CI) (CA INDEX NAME)



CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 31

IT 132628-70-7P 157485-05-7P
(preparation and mesylation of)
IT 157485-06-8P
(preparation and reductive cyclization of)
REData is temporarily unavailable.

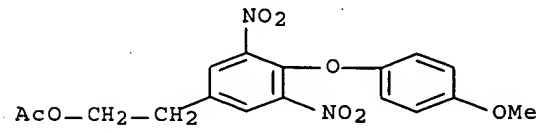
L37 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:28284 HCAPLUS Full-text
DOCUMENT NUMBER: 55:28284
ORIGINAL REFERENCE NO.: 55:5624g-i,5625a-i
TITLE: Enzymic conversion of iodinated thyronines to iodinated thyroacetic acids
AUTHOR(S): Tomita, Kenkichi; Lardy, Henry A.
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of Biological Chemistry (1960), 235, 3292-7
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:28284
ED Entered STN: 22 Apr 2001
AB cf. CA 51, 8172c; 53, 10527b. An extract of rat-kidney mitochondria, fortified with diphosphopyridine nucleotide (DPN), converts 3,5-diiodothyronine, 3'-iodothyronine, and uniodinated thyronine as well as thyroxine and triiodothyronine, to their corresponding AcOH analogs. Although thyronamine (I) is converted to thyroacetic acid (II), iodinated thyronamines are not; this finding indicates that they are not intermediates in the conversion of iodinated thyronines to AcOH analogs. Iodinated thyropyruvic acids and thyroacetaldehydes could not be detected as intermediates, but synthetic diiodothyropyruvic acid-2-C14 was converted to radioactive diiodothyroacetic acid. The synthesis and biol. activity of 3,3',5-triiodothyroethanol (III), 3,5-diiodothyroethanol (IV), and noniodinated thyroethanol (V) are described. These compds. were oxidized to their respective thyroacetic acid analogs by the kidney enzyme system. It is concluded that the enzymic conversion of iodinated thyronines to iodinated thyroacetic acids proceeds by way of iodinated thyropyruvic acids and thyroacetaldehydes. p-MeOC6H4CH2CO2H (100 g.) refluxed 10 hrs. with 250 ml. 48% HBr and the mixture evaporated in vacuo yielded 64-80 g. p-hydroxyphenylacetic acid (VI), m. 149-51°. VI (150 g.), 450 ml. absolute EtOH, and 8 ml. H2SO4 yielded 159 g. Et ester (VII), b1.5 156-7°. VII could be reduced with LiAlH4, but reduction with Na in BuOH gave a better yield. VII (90 g.) in 1 l. anhydrous BuOH treated with 60 g. Na yielded 53.7 g. tyrosol (VIII), m. 89-91°, dibenzoate m. 110-12°. VIII (69 g.), 150 ml. AcOH, and 1.15 ml. H2SO4 yielded 74.8 g. p-hydroxyphenethyl acetate (IX), b0.7 154-5.5°, m. 61-2°. IX (36 g.) added to 720 ml. H2SO4 in a bath at -25° to -30°, and the mixture treated dropwise with 62.5 ml. HNO3 (d. 1.4) below -10° gave 38.2 g. 4-hydroxy-3,5- dinitrophenethyl acetate (X), m. 91.5-2.5°. X (2.5 g.) and 10 ml. Ac2O containing 1 drop H2SO4 yielded dinitrotyrosyl diacetate. X (10.8 g.) and 8.4 g. p-MeC6H4SO2Cl in 16 ml. dry pyridine heated 30 min. (oil bath at 100-5°), 14.9 g. p-MeOC6H4OH added, the mixture refluxed 1 hr. (bath temperature 180°), cooled, dissolved in 75 ml. CHCl3, the solution washed and dried, evaporated in vacuo, the residue (11.4 g.) passed through Al2O3, 350 ml. eluate collected, and evaporated yielded 10.1 g. 2-[3,5-dinitro-4-(4-methoxyphenoxy)phenyl]ethyl acetate (XI), m. 110-11.5°. MeSO2Cl could also be used with the same yield. XI (2 g.) in 75 ml. absolute EtOH (ice-cold) treated with dry HCl, gave 1.59 g. 2-[3,5-dinitro-4-(4-methoxyphenoxy)phenyl]ethyl alc., m. 137-9°. XI (1 g.) in 100 ml. AcOH hydrogenated over 0.1 g. 10% Pd-C 1-2 hrs. at room temperature, the solution filtered, evaporated in vacuo at 40°, the residue heated 3 hrs. at 70-80° with 30 ml. Ac2O, treated with H2O, and evaporated in vacuo yielded 310 mg. 2-[N,N-diacetyl-3,5-diamino-4-(4-

methoxyphenoxy)phenyl]ethyl acetate (XII), m. 162-4°. XI (7.5 g.) in 100 ml. AcOH hydrogenated over 0.4 g. 10% Pd-C, the diamine tetrazotized, added to a mixture of 27 g. NaI, 15.2 g. iodine, and 300 ml. H2O which had been treated with 3.6 g. urea and 200 ml. CHCl3, the CHCl3 layer separated, the aqueous layer extracted with CHCl3, the combined exts. washed and dried, the CHCl3 evaporated, and the residue in 75 ml. C6H6 passed through Al2O3, yielded (from the 1st 100 ml. eluate) 7.3-8.5 g. 2-[3,5-diiodo-4-(4-methoxyphenoxy)phenyl]ethyl acetate (XIII), m. 108-10°. XIII (10 g.) refluxed 7 hrs. with 100 ml. AcOH and 100 ml. HI (b. 125-6°) containing 1 g. red P, the solution decanted, the P washed with H2O, the washings and the decanted solution mixed, cooled overnight, and the precipitate filtered off yielded 10 g. 2-[3,5-diiodo-4-(4- hydroxyphenoxy)phenyl]ethyl iodide (XIV), m. 166-8°. XIV (2 g.) in 30 ml. warm EtOH mixed with 30 ml. 2N NaOH, the mixture held 2 hrs. at room temperature, slightly acidified with HCl, diluted with H2O, and cooled overnight yielded (probably) 3,5-diiodo-4-(4- hydroxyphenoxy)styrene, m. 123-5°. XIV (5.92 g.) in 750 ml. AcOH treated with 3.34 g. AgOAc, yielded 4.5 g. 2-[3,5-diiodo-4-(4- hydroxyphenoxy)phenyl]ethyl acetate (XV), m. 146-8° (C6H6); after drying at 100° XV m. 152-4° without sintering. XV (1 g.) in 30 ml. EtOH treated with 30 ml. 2N NaOH yielded 0.9 g. 3,5-diiodothyroethanol (XVI), m. 185-7°. XVI (964 mg.) in 145 ml. EtOH and 48 ml. NH4OH treated dropwise (ice bath) with 4 ml. N iodine, the mixture allowed to stand 1 hr., evaporated in vacuo (40°), the residue in 60 ml. boiling EtOH diluted with 100 ml. H2O, and cooled overnight yielded III, sintered 160-5°, m. 186°. Attempts to prepare tetraiodothyroethanol yielded crystals m. about 200° which decomposed on crystallization XVI (1.5 mg.) in 2 ml. MeOH and 2 ml. NH4OH treated with 150 γ iodine-131 in cyclohexane, the mixture concentrated, extracted with BuOH, and the exts. evaporated in vacuo yielded 3,3',5-triiodothyroethanol-I131. 3,5- Diiodothyroacetic acid (1.5 g.) in a Soxhlet apparatus extracted into 1.5 g. LiAlH4 in 700 ml. Et2O, the mixture refluxed 72 hrs., treated with H2O, the Et2O decanted, the residue dissolved in a small amount of dilute H2SO4, extracted with Et2O, and the Et2O evaporated yielded V, m. 140-1.5°. XVI (40 mg.) in 15 ml. EtOH and 5 ml. NH4OH hydrogenated several hrs. at atmospheric pressure over W-2 Raney Ni (3 ml., about 1.8 g.), and the filtrate evaporated to dryness in vacuo yielded V, m. 141-2°, dibenzoate m. 119-21°. Com. triiodothyroacetic acid yielded 83% II, m. 189-91°. Com. DL-thyronine heated under H with Ph2NH yielded I, m. 135-7°.

IT 102026-43-7P, Phenethyl alcohol, 4-(p-methoxyphenoxy)-3,5-dinitro-, acetate
(preparation of)

RN 102026-43-7 HCAPLUS

CN Phenethyl alcohol, 4-(p-methoxyphenoxy)-3,5-dinitro-, acetate (6CI) (CA INDEX NAME)



CC 11A (Biological Chemistry: General)

IT 501-94-0P, Tyrosol 736-05-0P, Phenethyl alcohol, 4-(4-hydroxy-3-iodophenoxy)-3,5-diiodo- 790-55-6P, Phenethyl alcohol, 4-(p-hydroxyphenoxy)-3,5-diiodo- 92106-70-2P, Phenol, p-[2,6-diiodo-4-(2-iodoethyl)phenoxy]- 94575-19-6P, Phenethyl alcohol, 3,5-diiodo-4-(p-methoxyphenoxy)-, acetate 100970-36-3P, Phenethyl alcohol, 4-(p-methoxyphenoxy)-3,5-dinitro-

102026-43-7P, Phenethyl alcohol, 4-(p-methoxyphenoxy)-3,5-dinitro-, acetate 103162-72-7P, Phenethyl alcohol, p-(p-hydroxyphenoxy)-, dibenzoate 106422-15-5P, Phenethyl alcohol, p-(p-hydroxyphenoxy)- 111161-93-4P, Acetamide, N,N'-[5-(2-hydroxyethyl)-2-(p-methoxyphenoxy)-m-phenylene]bis-, acetate 132962-12-0P, Phenethyl alcohol, 4-(p-hydroxyphenoxy)-3,5-diiodo-, acetate
(preparation of)
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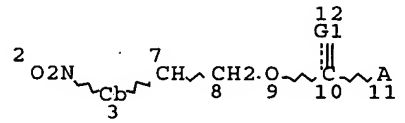

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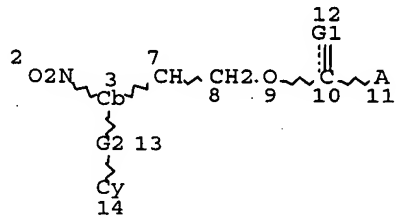

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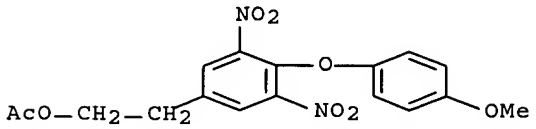
L42 ANSWER 1 OF 2 CAOLD COPYRIGHT 2007 ACS on STN
IT 102026-43-7
RN 102026-43-7 CAOLD
CN Phenethyl alcohol, 4-(p-methoxyphenoxy)-3,5-dinitro-, acetate (6CI) (CA INDEX NAME)



L42 ANSWER 2 OF 2 CAOLD COPYRIGHT 2007 ACS on STN
IT 101351-56-8
RN 101351-56-8 CAOLD
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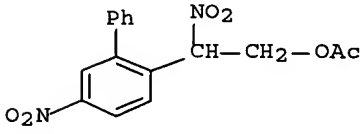

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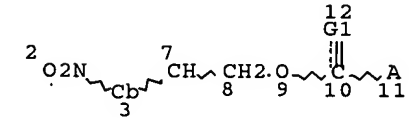

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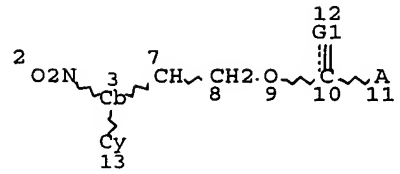

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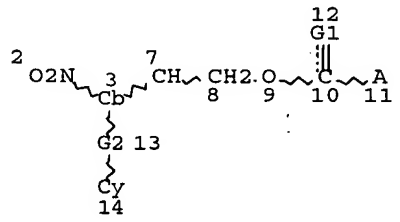

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L28 84 SEA FILE=REGISTRY SUB=L6 SSS FUL L25
L31 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L28
L32 46 SEA FILE=HCAPLUS ABB=ON PLU=ON BUEHLER, S?/AU
L33 406 SEA FILE=HCAPLUS ABB=ON PLU=ON OTT, M?/AU
L34 934 SEA FILE=HCAPLUS ABB=ON PLU=ON PFLEIDERER, W?/AU
L35 5 SEA FILE=HCAPLUS ABB=ON PLU=ON (L32 OR L33 OR L34) AND (L16 OR L31)
L36 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L35
L37 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 NOT (L35 OR L36)
L44 3 SEA FILE=HCAPLUS ABB=ON PLU=ON ("CA52:17177B"/OREF OR

"CA55:5624H"/OREF)
L45 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 NOT ((L35 OR L36 OR L37))

=> d l45 1-2 all
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L45 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1958:97742 HCAPLUS Full-text
DN 52:97742
OREF 52:17177b-f
ED Entered STN: 22 Apr 2001
TI Stilbenes. XV. Addition of acetyl nitrate to stilbenes
AU Drefahl, Gunther; Crahmer, Heinz
CS Univ. Jena, Germany
SO Chemische Berichte (1958), 91, 745-50
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
CC 10E (Organic Chemistry: Benzene Derivatives)
OS CASREACT 52:97742
AB cf. preceding abstract To a cold, solidified mixture of 2 g. stilbene (I) in 20 g. glacial AcOH (II) was added dropwise with stirring a mixture of 1.2 cc. HNO3 (d. 1.4) and 3 cc. H2SO4, kept 2 hrs. not above 20° and poured on ice, giving 50-60 mg. 4-NO2 derivative of I, m. 157°. I (2 g.) in 20 cc. II with 2 cc. HNO3 (d. 1.502) and 3 cc. H2SO4 kept 2 hrs. at 25° and poured on ice gave 0.1 g. 4,4'-di-NO2 derivative of I, m. 290°. To 2 g. I in 20 cc. Ac2O at -10°, kept free from moisture were added very slowly within 1 hr., 5 g. freshly distilled acetyl nitrate, (the temperature kept below -8°), allowed to stand 1 hr., poured on ice, and filtered after 10 hrs. to give 60 mg. 2,2'-di-NO2 derivative of I, m. 192°. trans-I (5 g.), suspended in 25 cc. II and 30 cc. Ac2O, stirred at 0° to 5° with 2.5 g. each of HNO3 and II, kept 1 hr. at 15°, and poured on ice, gave 45% DL-threo-2-nitro-1-acetoxy-1,2- diphenylethane, m. 135° (AcOH, followed by EtOH), 1 g. of which in 150 cc. AcOEt, hydrogenated with 0.2 g. Raney Ni, gave 80% DL-threo-2-acetamido-1,2-diphenylethanol (III), m. 155°; this with Ac2O gave O,N-diacetyl-DL-isodiphenylhydroxyethylamine, m. 118° (cf. Read, et al., C.A. 24, 609). α-Me derivative of I (4 g.) in 20 cc. Ac2O and 15 cc. II, stirred with 4 g. HNO3 (d. 1.458) at 0°-5° gave 35% DL-threo-2-nitro-1-acetoxy-1-methyl- 1,2-diphenylethane, m. 106° (II, followed by EtOH), which when hydrogenated with Ni gave 60% 1-Me derivative (IV) of III, m. 186.5° (dilute EtOH). DL-erythro-2-Amino-1-methyl-1,2- diphenylethanol-HCl was formed by the McKenzie and Barrow method (C.A. 7, 3486) and heated 15 min. at 150° with HCONH2, giving 82% formyl derivative MeCPh(OH)CHPhNHCHO, m. 159° (dilute EtOH), 0.7 g. of which at 5° in 3 cc. SOCl2 was warmed to 25°, treated with ice and then refluxed 90 min., giving a clear solution from which NaOH precipitated 56% DL-threo-2-amino-1-methyl-1,2-diphenylethanol, m. 94-5° (petr. ether); this with Ac2O gave IV.
IT Addition reactions
Addition reactions
(of acetyl nitrate with stilbenes)
IT 588-59-0, Stilbene
(derivs.)
IT 888-33-5P, 2-Propanol, 1-amino-1,2-diphenyl-, DL-threo- 2501-02-2P, Stilbene, 4,4'-dinitro- 6275-02-1P, Stilbene, 2,2'-dinitro- 51507-26-7P, 2-Propanol, 1-nitro-1,2-diphenyl-, DL-threo-, acetate 56184-93-1P, Ethanol, 2-nitro-1,2-diphenyl-, DL-threo-, acetate 84388-60-3P, Acetamide, N-(2-hydroxy-1,2-diphenylethyl)-, DL-threo-

108976-11-0P, Acetamide, N-(2-hydroxy-1,2-diphenylpropyl)-, DL-threo-
860215-81-2P, Formamide, N-(2-hydroxy-1,2-diphenylpropyl)-
(preparation of)
IT 4003-94-5, Stilbene, 4-nitro-
(reaction with acetyl nitrate)
IT 591-09-3, Acetyl nitrate
(reaction with stilbenes)

L45 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1958:97741 HCAPLUS Full-text
DN 52:97741
OREF 52:17176h-i,17177a-b
ED Entered STN: 22 Apr 2001
TI Investigations with stilbene. XIV. Analytical use of 4-stilbenylnitrosohydroxylamine, "styrylcupferron"
AU Drefahl, Gunther; Geissler, Arthur
CS Friedrich-Schiller Univ., Jena, Germany
SO Fresenius' Zeitschrift fuer Analytische Chemie (1958), 160, 34-8
CODEN: ZACFAU; ISSN: 0016-1152
DT Journal
LA Unavailable
CC 10E (Organic Chemistry: Benzene Derivatives)
AB cf. C.A. 52, 16285h. Free 4-nitrostilbenylnitrosohydroxylamine (I) is not stable, but the HOEtNH2 salt (II) of I is stable for long periods of time. When the Na salt of I is suspended in 2N HCl at 0° and the I is extracted into Et2O, HOEtNH2 ppts. II, yellow crystals, m. 251° (H2O). A 0.5-1% solution of II is prepared by adding II to boiling H2O and filtering. This solution is not stable. Cu++ yields a greenish gray precipitate from warm NH3 solns. The precipitate can be easily filtered off, washed, dried 40 min. at 110°, and weighed. It has the composition C28H22O4N4Cu, it is soluble in warm organic solvents, and is decomposed by mineral acids. From a neutral solution containing 15% iso-PrOH at 60°, Fe+++ yields a brown flocculent precipitate whose composition, after washing with hot H2O (70°) and drying 40 min. at 110°, is C42H33O6N6Fe. The complex is soluble in organic solvents, stable toward HOAc, and decomposed by mineral acids. Al+++ is precipitated by II as C42H33O6N6Al from neutral solution If aqueous II is added to neutral Al, the H+ released is neutralized with 4:1 EtOH-C5H5N. If the precipitation is started in ammoniacal-tartrate solution, neutralization is done with NH4Cl. The Al complex is soluble in organic solvents and decomposed by acids. The determination of Al, Fe, and Cu as complexes of II gives excellent recoveries.
IT Analysis
(N-nitroso-N-p-styrylphenylhydroxylamine in gravimetric)
IT Cupferron, styryl-
IT Aluminum, compound with N-nitroso-N-p-styrylphenylhydroxyl-amine
(in Al determination)
IT Iron, compound with N-nitroso-N-p-styrylphenylhydroxylamine
(in Fe determination)
IT 7429-90-5, Aluminum 7439-89-6, Iron 7440-50-8, Copper
(analysis, determination, N-nitroso-N-p-styrylphenylhydroxylamine in)
IT 100872-28-4, Hydroxylamine, N-nitroso-N-p-styrylphenyl- 101424-32-2, Hydroxylamine, N-nitroso-N-p-styrylphenyl-, compound with 2-aminoethanol
(and metal derivs.)
IT 588-59-0, Stilbene
(derivs.)
IT 7440-50-8, Copper, compounds, with N-nitroso-N-p-styrylphenylhydroxylamine
(in Cu determination)
IT 21471-69-2P, Benzamide, N-(1,2-diphenylpropyl)- 101424-32-2P, Ethanol, 2-amino-, compound with N-nitroso-N-p-styrylphenylhydroxyl-amine

(preparation of)

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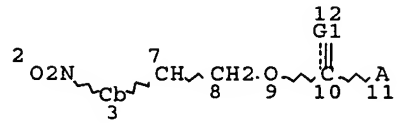


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DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
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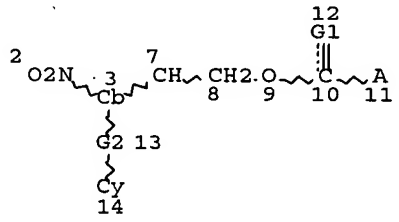


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REP G2=(0-10) A
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NSPEC    IS RC     AT  11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   10

STEREO ATTRIBUTES: NONE
L28           84 SEA FILE=REGISTRY SUB=L6 SSS FUL L25
L43            5 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L28


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YOU HAVE REQUESTED DATA FROM FILE 'BEILSTEIN' - CONTINUE? (Y)/N:y
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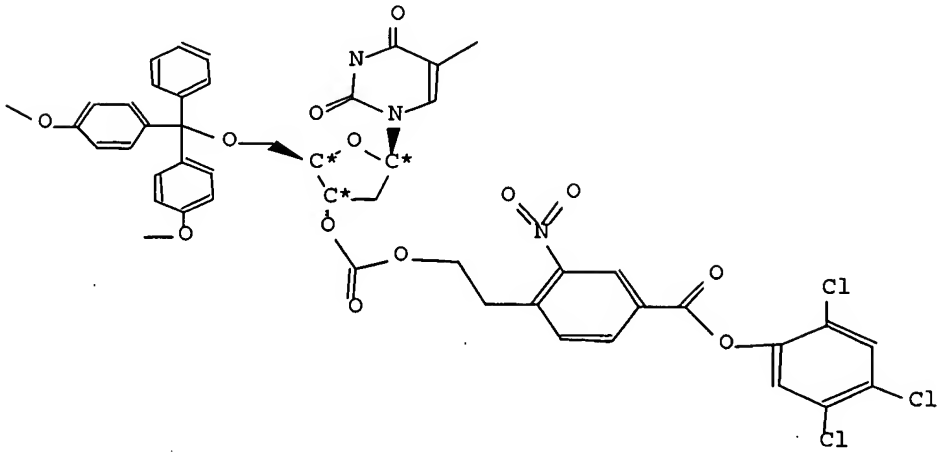
L43 ANSWER 1 OF 5 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4347896
Beilstein Pref. RN (BPR):	134403-95-5
CAS Reg. No. (RN):	**134403-95-5**
Chemical Name (CN):	4-<2,3'-(5'-O-4,4'-dimethoxytrityl-thymidyl)carbonyloxyethyl>-3-nitrobenzoate 2,4,5-trichlorophenyl ester
Autonom Name (AUN):	4-(2-<2-<bis-(4-methoxy-phenyl)-phenyl-methoxymethyl>-5-(5-methyl-2,4-dioxo-3,4-dihydro-2H-pyrimidin-1-yl)-tetrahydro-furan-3-yloxycarbonyloxy>-ethyl)-3-nitro-benzoic acid 2,4,5-trichloro-phenyl ester
Molec. Formula (MF):	C47 H40 Cl3 N3 O13
Molecular Weight (MW):	961.20
Lawson Number (LN):	28796, 20545, 11705, 6582, 5222, 1762, 289
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	3938264
Tautomer ID (TAUTID):	4218627
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1992/07/20
Update Date (DUPD):	1994/02/03



Field Availability:

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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1

AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	7
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

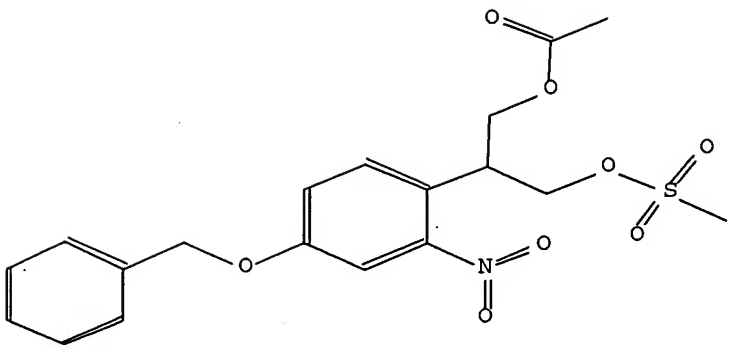
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Eritja, Ramon; Robles, Jordi; Avino, Anna; Albericio, Fernando; Pedroso, Enrique, Tetrahedron, CODEN: TETRAB, 48(20), <1992>, 4171-4182; BABS-5648369
2. Eritja, Ramon; Robles, Jordi; Fernandez-Forner, Dolors; Albericio, Fernando; Giralt, Ernest; Pedroso, Enrique, Tetrahedron Lett., CODEN: TELEAY, 32(11), <1991>, 1511-1514; BABS-5539921

L43 ANSWER 2 OF 5 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4338576
Beilstein Pref. RN (BPR):	132628-57-0
CAS Reg. No. (RN):	132628-57-0
Chemical Name (CN):	3-acetoxy-2-(4-benzyloxy-2-nitrophenyl)propan-1-yl methanesulfonate
Autonom Name (AUN):	acetic acid 2-(4-benzyloxy-2-nitro-phenyl)-3-methanesulfonyloxy-propyl ester
Molec. Formula (MF):	C19 H21 N O8 S
Molecular Weight (MW):	423.44
Lawson Number (LN):	6417, 5228, 2705, 1155
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	3919268
Tautomer ID (TAUTID):	4214413
Beilstein Citation (BSO):	6-06
Entry Date (DED):	1992/07/20
Update Date (DUPD):	1995/05/11



Field Availability:

Code	Name	Occurrence
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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

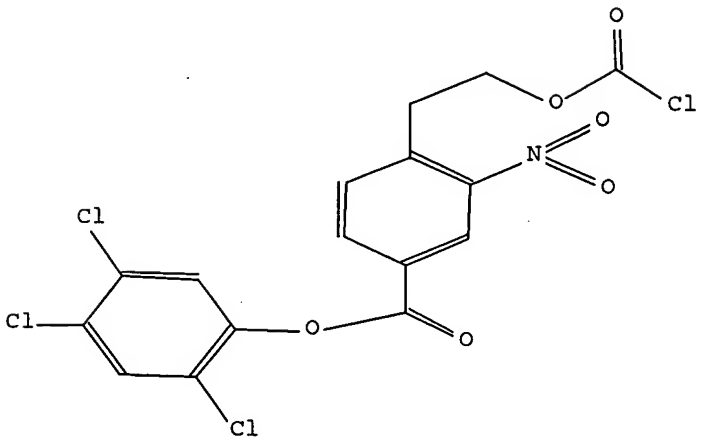
Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Fukuda, Yasumichi; Itoh, Yoshio; Nakatani, Kazuhiko; Terashima, Shiro, Tetrahedron, CODEN: TETRAB, 50(9), <1994>, 2793-2808; BABS-5850464
2. Fukuda, Yasumichi; Nakatani, Kazuhiko; Ito, Yoshio; Terashima, Shiro, Tetrahedron Lett., CODEN: TELEAY, 31(46), <1990>, 6699-6702; BABS-5540762

L43 ANSWER 3 OF 5 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4337714
Beilstein Pref. RN (BPR):	134403-92-2
CAS Reg. No. (RN):	134403-92-2
Molec. Formula (MF):	C16 H9 Cl4 N O6
Molecular Weight (MW):	453.06
Lawson Number (LN):	11705, 5222, 1762
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	3924539
Tautomer ID (TAUTID):	4207014
Beilstein Citation (BSO):	6-10
Entry Date (DED):	1992/07/20
Update Date (DUPD):	1994/02/03



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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence

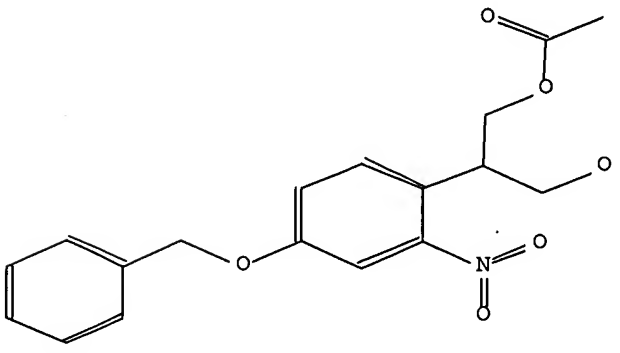
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Eritja, Ramon; Robles, Jordi; Avino, Anna; Albericio, Fernando; Pedroso, Enrique, Tetrahedron, CODEN: TETRAB, 48(20), <1992>, 4171-4182; BABS-5648369
2. Eritja, Ramon; Robles, Jordi; Fernandez-Forner, Dolors; Albericio, Fernando; Giralt, Ernest; Pedroso, Enrique, Tetrahedron Lett., CODEN: TELEAY, 32(11), <1991>, 1511-1514; BABS-5539921

L43 ANSWER 4 OF 5 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4332423
Beilstein Pref. RN (BPR):	132628-56-9
CAS Reg. No. (RN):	132628-56-9
Chemical Name (CN):	3-acetoxy-2-(4-benzyloxy-2-nitrophenyl)propan-1-ol
Autonom Name (AUN):	acetic acid 2-(4-benzyloxy-2-nitro-phenyl)-3-hydroxy-propyl ester
Molec. Formula (MF):	C18 H19 N O6
Molecular Weight (MW):	345.35
Lawson Number (LN):	6417, 5228, 1155
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	3914827
Tautomer ID (TAUTID):	4209143
Beilstein Citation (BSO):	6-06
Entry Date (DED):	1992/07/20
Update Date (DUPD):	1995/05/11



Field Availability:

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BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

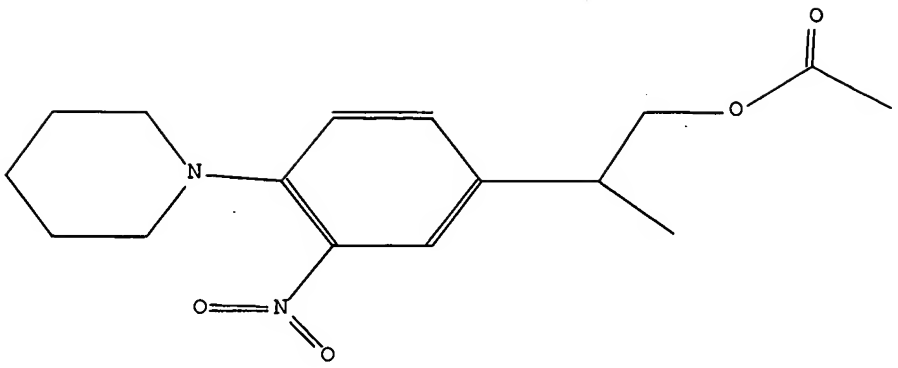
Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Fukuda, Yasumichi; Itoh, Yoshio; Nakatani, Kazuhiko; Terashima, Shiro, Tetrahedron, CODEN: TETRAB, 50(9), <1994>, 2793-2808; BABS-5850464
2. Fukuda, Yasumichi; Nakatani, Kazuhiko; Ito, Yoshio; Terashima, Shiro, Tetrahedron Lett., CODEN: TELEAY, 31(46), <1990>, 6699-6702; BABS-5540762

L43 ANSWER 5 OF 5 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1592959
Beilstein Pref. RN (BPR):	31872-50-1
CAS Reg. No. (RN):	31872-50-1
Chemical Name (CN):	acetic acid 2-(3-nitro-4-piperidin-1-yl-phenyl)-propyl ester
Autonom Name (AUN):	acetic acid 2-(3-nitro-4-piperidin-1-yl-phenyl)-propyl ester
Molec. Formula (MF):	C16 H22 N2 O4
Molecular Weight (MW):	306.36
Lawson Number (LN):	24081, 14913, 1155
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1443981
Tautomer ID (TAUTID):	1496690
Beilstein Citation (BSO):	5-20
Entry Date (DED):	1988/11/30
Update Date (DUPD):	1988/12/08



Field Availability:

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RN	CAS Registry Number	1
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AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
BP	Boiling Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Patent: Merck US 1212149 1970, Chem.Abstr., 74(141542)

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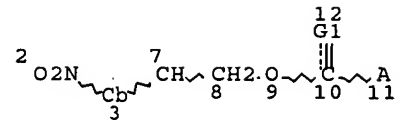


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
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L8                STR
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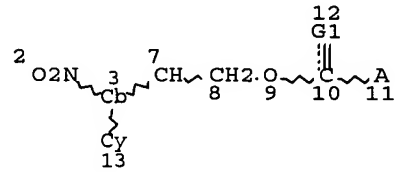


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
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L16            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10
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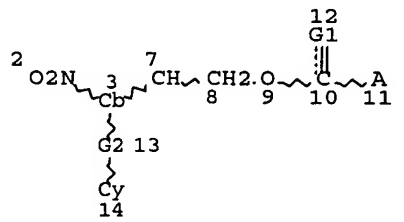

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
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L31          28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28
L32          46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BUEHLER, S?/AU
L33         406 SEA FILE=HCAPLUS ABB=ON  PLU=ON  OTT, M?/AU
L34         934 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PFLEIDERER, W?/AU
L35           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L32 OR L33 OR L34) AND
                (L16 OR L31)


=> d l35 1-4 ibib ed abs fhitstr hitind
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y



L35  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:483932  HCAPLUS  Full-text
DOCUMENT NUMBER:          145:124806
TITLE:                    Highly efficient photolabile protecting groups
                          with intramolecular energy transfer
AUTHOR(S):                Woell, Dominik; Smirnova, Julia; Pfleiderer,
                          Wolfgang; Steiner, Ulrich E.
CORPORATE SOURCE:         Fachbereich Chemie, Universitaet Konstanz,
                          Konstanz, 78464, Germany
SOURCE:                   Angewandte Chemie, International Edition (2006),
                          45(18), 2975-2978
                          CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER:                Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
ED   Entered STN:  24 May 2006
AB   A series of novel, highly light-sensitive photolabile protecting groups for
     light-controlled DNA synthesis has been developed.  In these compds. the NPPOC
     (nitrophenylpropoxycarbonyl) protecting group is covalently linked to
     thioxanthone as an intramol. antenna.  The photochem. kinetics of these
     compds. under stationary irradiation conditions has been quant. investigated,
     and photochem. quantum yields as well as chemical yields of the
     photodeprotected substrate were determined for thymidine as a model substrate.
     The kinetics of triplet-triplet energy transfer between the antenna mol. and
     the photolabile protecting group has been investigated by laser flash
     spectroscopy. Besides triplet-triplet energy transfer, a sensitization
     mechanism involving the excited sensitizer singlet must be also involved,
     particularly in the systems with short linkers.  The high light sensitivity of
     these protecting groups should allow their use in photolithog. synthesis of
     high-d. DNA chips.
IT   777864-75-2
       (highly efficient photolabile protecting groups for applications in
       photolithog. synthesis of high-d. DNA chips)
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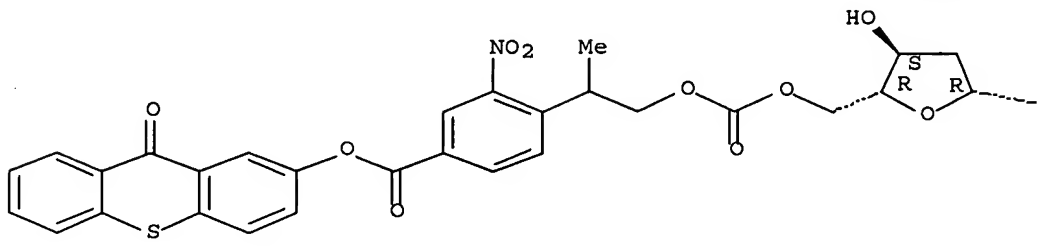
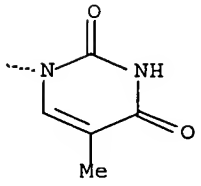
RN 777864-75-2 HCAPLUS
CN Thymidine, 5'-[2-[2-nitro-4-[[(9-oxo-9H-thioxanthen-2-yl)oxy]carbonyl]phenyl]propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

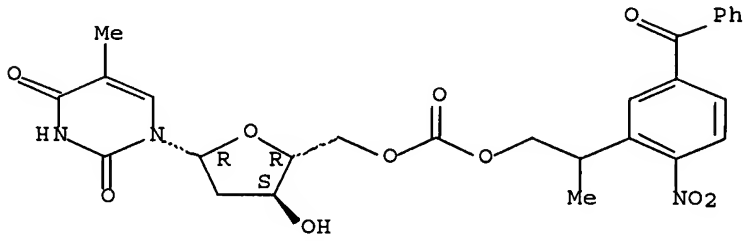


CC 33-9 (Carbohydrates)
Section cross-reference(s): 3
IT 50-89-5D, Thymidine, 5'-blocked with photolabile protecting groups
189216-59-9 777864-69-4 **777864-75-2** 777864-78-5
855743-25-8 855743-26-9 855743-29-2
(highly efficient photolabile protecting groups for applications in photolithog. synthesis of high-d. DNA chips)
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1151413 HCAPLUS Full-text
DOCUMENT NUMBER: 145:397718
TITLE: Recent highlights on photolytic oligonucleotide array in situ synthesis
AUTHOR(S): Stengele, Klaus-Peter; Buehler, Jochen; **Buehler, Sigrid**; Kvassiouk, Evgueni; Green, Roland; Prykota, Tamara; **Pfleiderer, Wolfgang**
CORPORATE SOURCE: Chemogenix GmbH, Waldkraiburg, Germany
SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2005), 24(5-7), 891-896
CODEN: NNNAFY; ISSN: 1525-7770
PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 Oct 2005
AB Light directed synthesis of high-d. oligonucleotide micro-arrays is currently performed using either ortho-nitro-benzyl-type [MeNPOC] or ortho-nitrophenyl-ethyl-type [NPPOC] protecting groups as the 5'-O-carbonate ester of the phosphoramidite building block. The synthesis cycle uses a combinatorial approach attaching one specific base per cycle, thus as many as 100 cycles need to be run to make an array of 25-mers. Time needed for deprotection/activation of the growing oligo chain dets. overall manufacturing time and consequently also cost. In this report we demonstrate the development of photo-protected phosphoramidite monomers for light directed array synthesis with increasing sensitivity to the UV light used. If combined with mask-less array synthesis, this technol. allows for synthesis of arrays with >780,000 different 25-mer oligonucleotides in about one hour and allows for high flexibility in array design and reiterative redesign. The arrays synthesized show high quality and reproducibility in our standard hybridization based assay.
IT **748789-44-8P**
(recent highlights on photolytic oligonucleotide array in situ synthesis)
RN 748789-44-8 HCAPLUS
CN Thymidine, 5'-[2-(5-benzoyl-2-nitrophenyl)propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-9 (Carbohydrates)
Section cross-reference(s): 22
IT 189216-59-9P **748789-44-8P** 868157-70-4P **868157-71-5P**
(recent highlights on photolytic oligonucleotide array in situ synthesis)
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:410525 HCAPLUS Full-text
DOCUMENT NUMBER: 143:78409
TITLE: Synthesis of caged nucleosides with photoremovable protecting groups linked to intramolecular antennae
AUTHOR(S): Smirnova, Joulia; Woell, Dominik; **Pfleiderer, Wolfgang**; Steiner, Ulrich E.
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Konstanz, Konstanz, D-78457, Germany

SOURCE: Helvetica Chimica Acta (2005), 88(4), 891-904
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:78409
ED Entered STN: 13 May 2005

AB Based on the [2-(2-nitrophenyl)propoxy]carbonyl (nppoc) group, six new photolabile protecting groups, each covalently linked to a 9H-thioxanthen-9-one (Tx) unit functioning as an intramol. triplet sensitizer, were synthesized. Linkers were introduced between the Me group or the aromatic ring of nppoc and the 2-position of Tx by means of classical organic synthesis combined with Pd catalyzed C-C coupling reactions. The new photolabile protecting groups to be used in light-directed synthesis of DNA chips were attached to the 5'-O-atom of thymidine via a carbonate linkage, giving rise to the desired caged nucleosides.

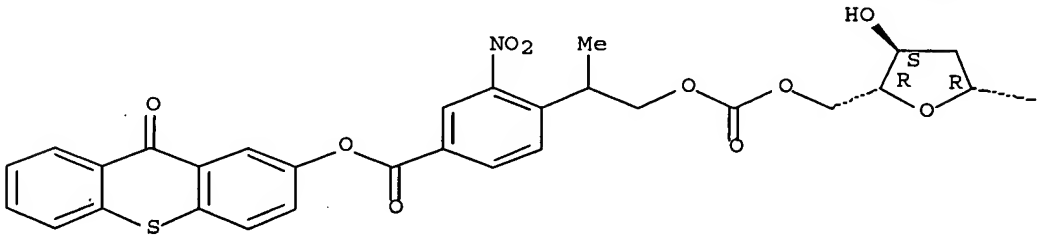
IT 777864-75-2P
(synthesis of caged nucleosides with photoremovable protecting groups linked to intramol. antennae)

RN 777864-75-2 HCAPLUS

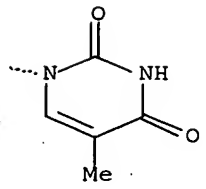
CN Thymidine, 5'-[2-[2-nitro-4-[[(9-oxo-9H-thioxanthen-2-yl)oxy]carbonyl]phenyl]propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 33-9 (Carbohydrates)

IT 50-89-5P, Thymidine, preparation 777864-69-4P 777864-75-2P 777864-78-5P 855743-25-8P 855743-29-2P
(synthesis of caged nucleosides with photoremovable protecting groups linked to intramol. antennae)

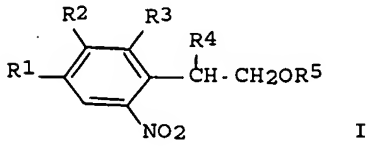
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:718549 HCAPLUS Full-text
DOCUMENT NUMBER: 141:225775
TITLE: Novel photolabile protective groups for improved processes to prepare oligonucleotide arrays
INVENTOR(S): **Buehler, Sigrid; Ott, Markus; Pfleiderer, Wolfgang**
PATENT ASSIGNEE(S): Nigu Chemie G.m.b.H., Germany
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004074300	A2	20040902	WO 2004-EP50158		20040219
WO 2004074300	A3	20041229			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2004175741	A1	20040909	US 2004-764989		20040126
GB 2414237	A	20051123	GB 2005-17834		20040219
PRIORITY APPLN. INFO.:			US 2003-449070P	P	20030221
			US 2004-764989	A	20040126
			WO 2004-EP50158	W	20040219

OTHER SOURCE(S): CASREACT 141:225775; MARPAT 141:225775
ED Entered STN: 02 Sep 2004
GI



I

AB The present invention discloses novel and improved nucleosidic and nucleotidic compds. I, wherein R1 is COOY, wherein Y is alkyl under the proviso that R2 is H, NO2, CN, OCH3, halogen, alkyl, alkoxyl; or R1 is H, NO2, CN, OCH3, halogen, alkyl, alkoxyl, under the proviso that R2 is aryl, heteroaryl, aroyl; R3 is H,

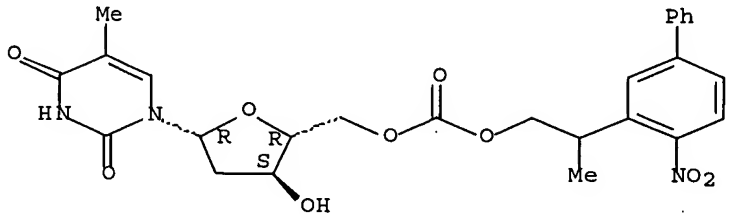
NO2, halogen; R4 is H, OCH3, alkyl; R5 is H, C(:X)Z; X is oxygen, sulfur; Z is leaving group, O-atom of a hydroxy group, or a N-atom of an amino group, of a compound comprising the photolabile protective group, that are useful in the light-directed synthesis of oligonucleotides, as well as, methods and reagents for their preparation These compds. are characterized by novel photolabile protective groups that are attached to either the 5'- or the 3'- hydroxyl group of a nucleoside moiety. The photolabile protective group is comprised of a 2-(2-nitrophenyl)-ethoxycarbonyl skeleton with at least one substituent on the aromatic ring that is either an aryl, an aroyl, a heteroaryl or an alkoxycarbonyl group. The present invention includes the use of the aforementioned compds. in light-directed oligonucleotide synthesis, the resp. assembly of nucleic acid micro-arrays and their application. Thus, N6-benzoyl-5'-O-[2-(5-benzoyl-2-nitrophenyl)-1-propyloxycarbonyl]-2'-deoxyadenosine-3'-O-(3-cyanoethoxy-N,N-diisopropyl)phosphoramidite was prepared using 2-(2-nitrophenyl)-ethoxycarbonyl protective groups.

IT **702643-76-3P**
(2-(2-nitrophenyl)-ethoxycarbonyl novel photolabile protective groups for improved processes to prepare oligonucleotide arrays)

RN 702643-76-3 HCAPLUS

CN Thymidine, 5'-[2-(4-nitro[1,1'-biphenyl]-3-yl)propyl carbonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H

CC 33-10 (Carbohydrates)

IT 612-22-6P 31680-58-7P 36680-46-3P 51279-01-7P 51885-79-1P
148582-37-0P 189216-59-9P 275795-11-4P 335201-49-5P
335201-53-1P 702642-46-4P 702642-56-6P 702642-66-8P
702642-85-1P 702642-87-3P 702642-98-6P 702643-06-9P
702643-08-1P **702643-76-3P** 702643-86-5P 702643-87-6P
702644-26-6P 748789-25-5P 748789-26-6P 748789-27-7P
748789-28-8P **748789-29-9P** 748789-31-3P
748789-32-4P **748789-33-5P** **748789-34-6P**
748789-35-7P **748789-42-6P** **748789-43-7P**
748789-44-8P **748789-46-0P** **748789-47-1P**
748789-48-2P
(2-(2-nitrophenyl)-ethoxycarbonyl novel photolabile protective groups for improved processes to prepare oligonucleotide arrays)

IT **748789-30-2P** **748789-36-8P** **748789-37-9P**
748789-38-0P **748789-39-1P** **748789-40-4P**
748789-41-5P
(2-(2-nitrophenyl)-ethoxycarbonyl novel photolabile protective groups for improved processes to prepare oligonucleotide arrays)